The EPA CompTox Chemistry Dashboard - a centralized hub for integrating data for the environmental sciences

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National Center for Computational Toxicology

July 27th, 2017

What we are out to achieve…

- Tens of thousands of chemicals are of interest to a broad spectrum of stakeholders and the Agency.
- The National Center for Computational Toxicology is looking to integrate and share our data to support computational toxicology
- Chemical structures and data are required to develop prediction models
- Data should be accessible and *Open*

How we are getting there…

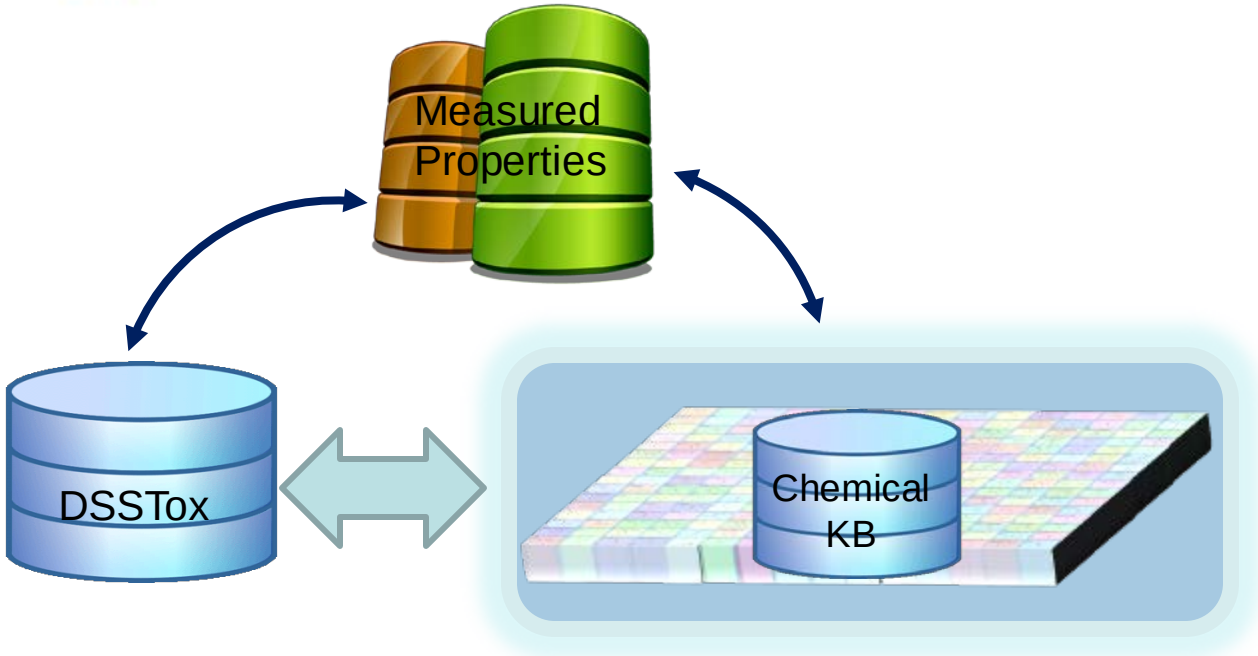
- Develop a publicly accessible web-based application
- Provide access to integrated data for ~750,000 chemicals – structures, properties, models, links to other agency resources
- Deliver search results to support different research needs

What we get as an outcome…

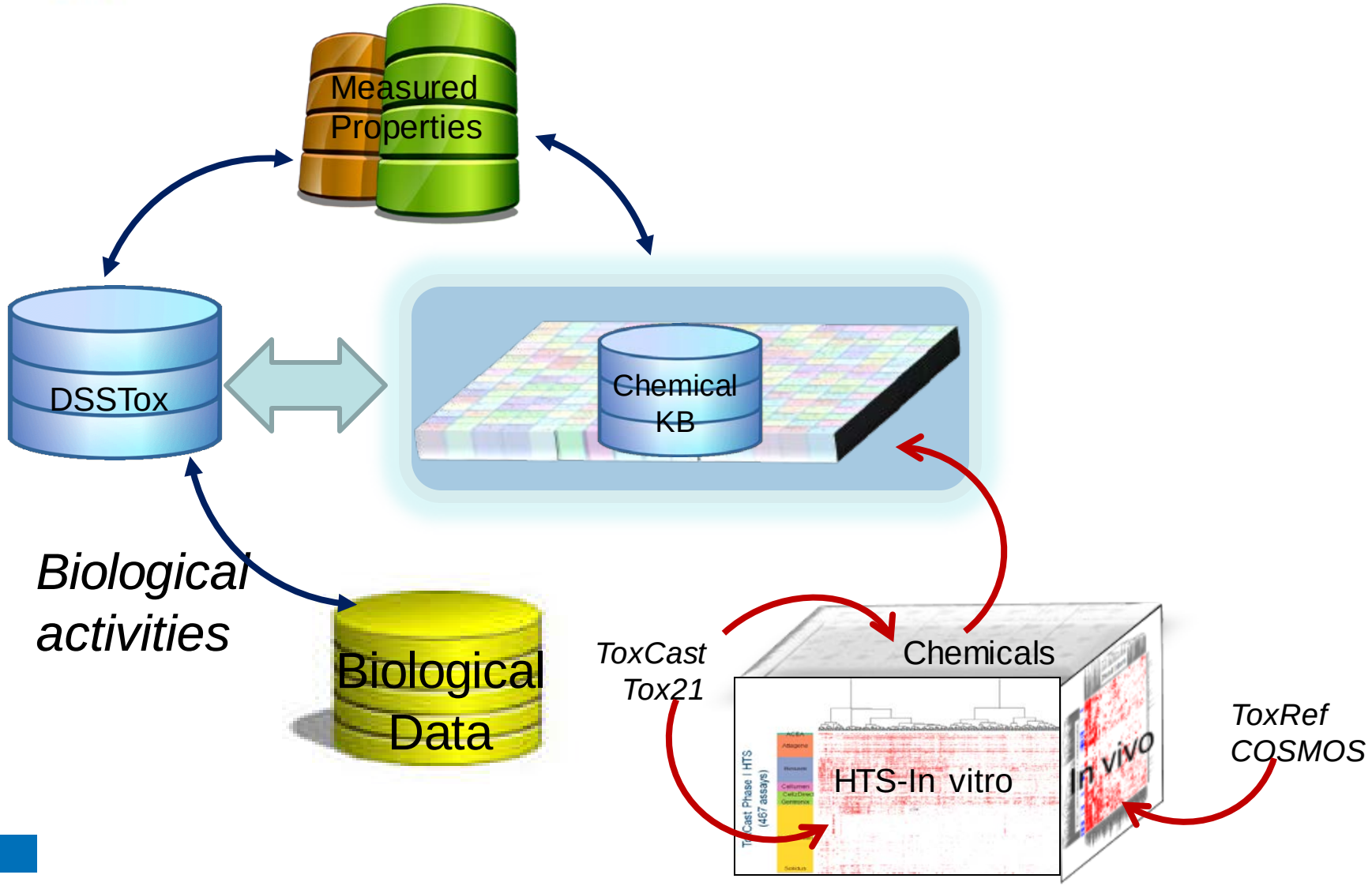
- Data are being used to:
  - Access toxicity data
  - Build prediction models
  - Speed chemical identification
  - Support additional software applications

- Open data allows for:
  - Integration via other public websites
  - Phone and tablet mobile applications

Chemically Integrated Data



Chemically Integrated Data



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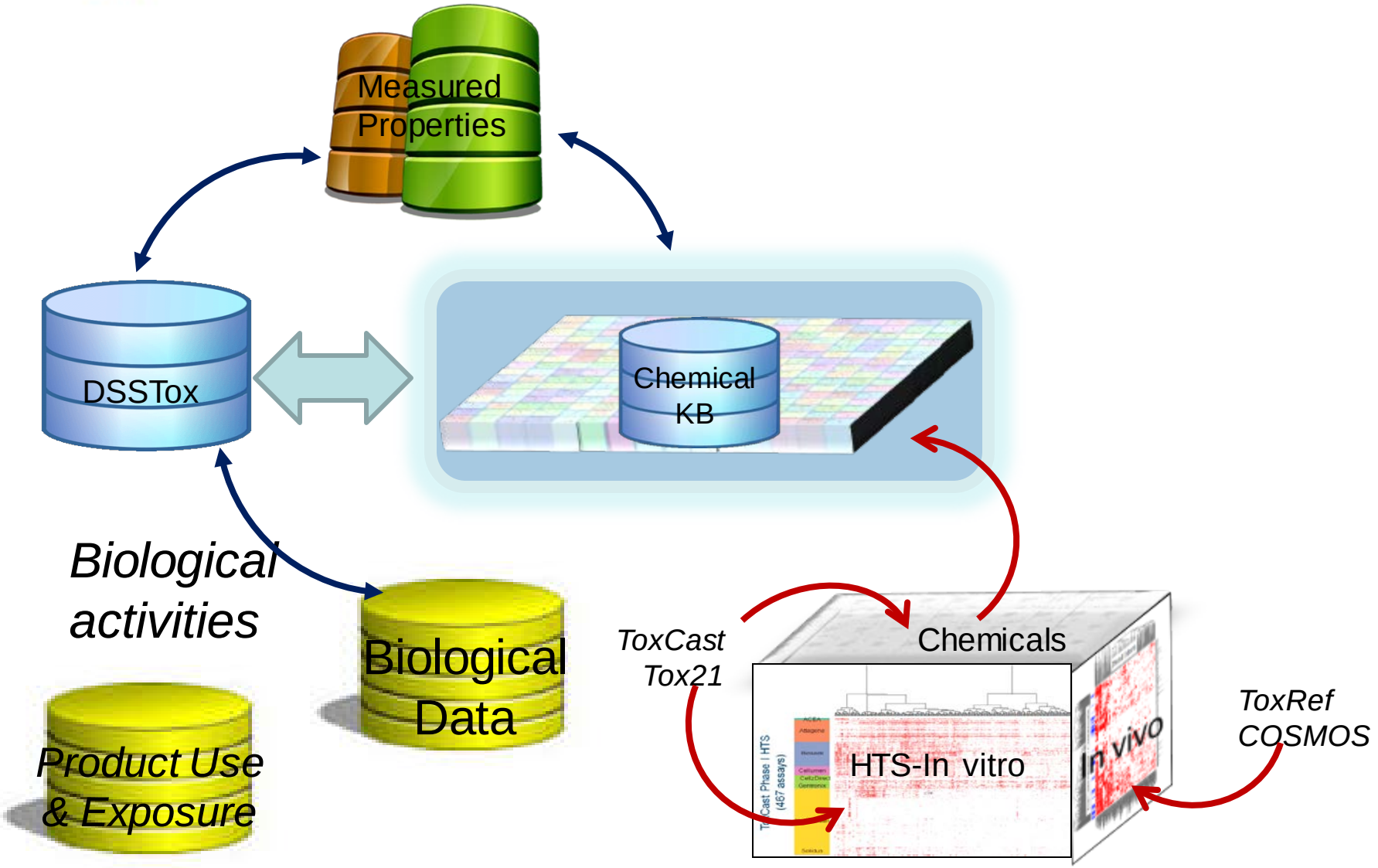
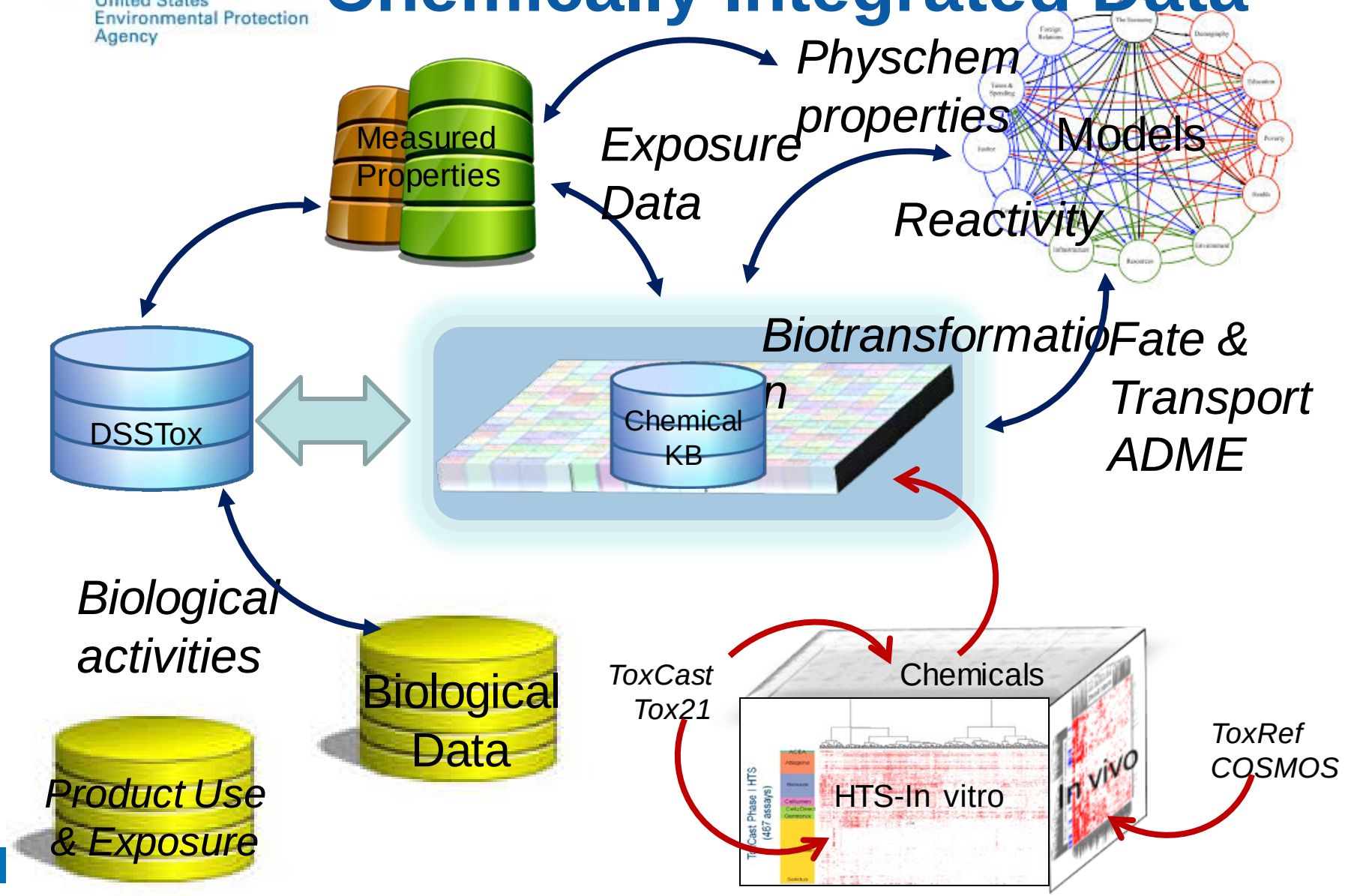
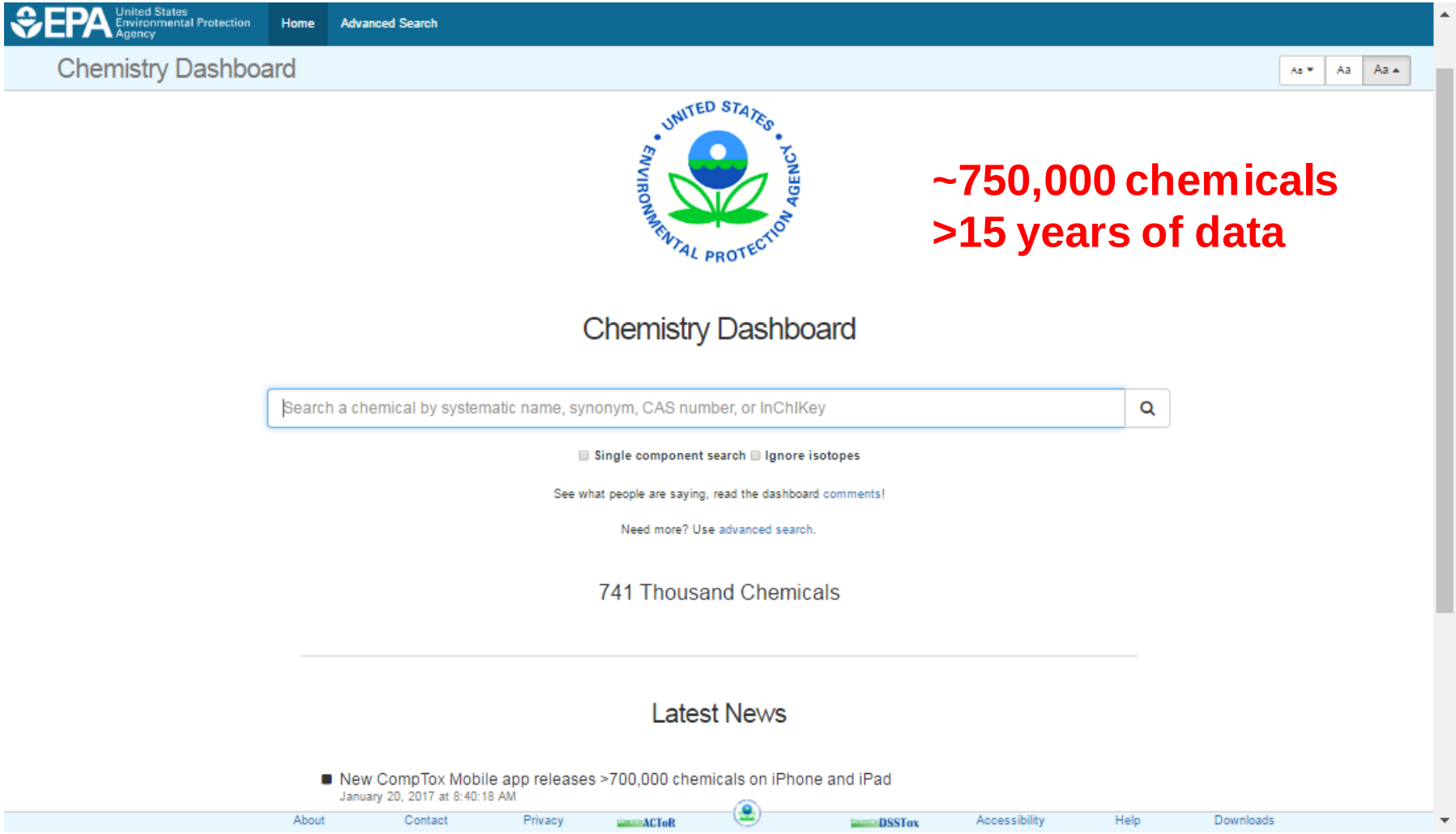


Chemically Integrated Data



Comptox Chemistry Dashboard

https://comptox.epa.gov



~750,000 chemicals
>15 years of data

Comptox Chemistry Dashboard

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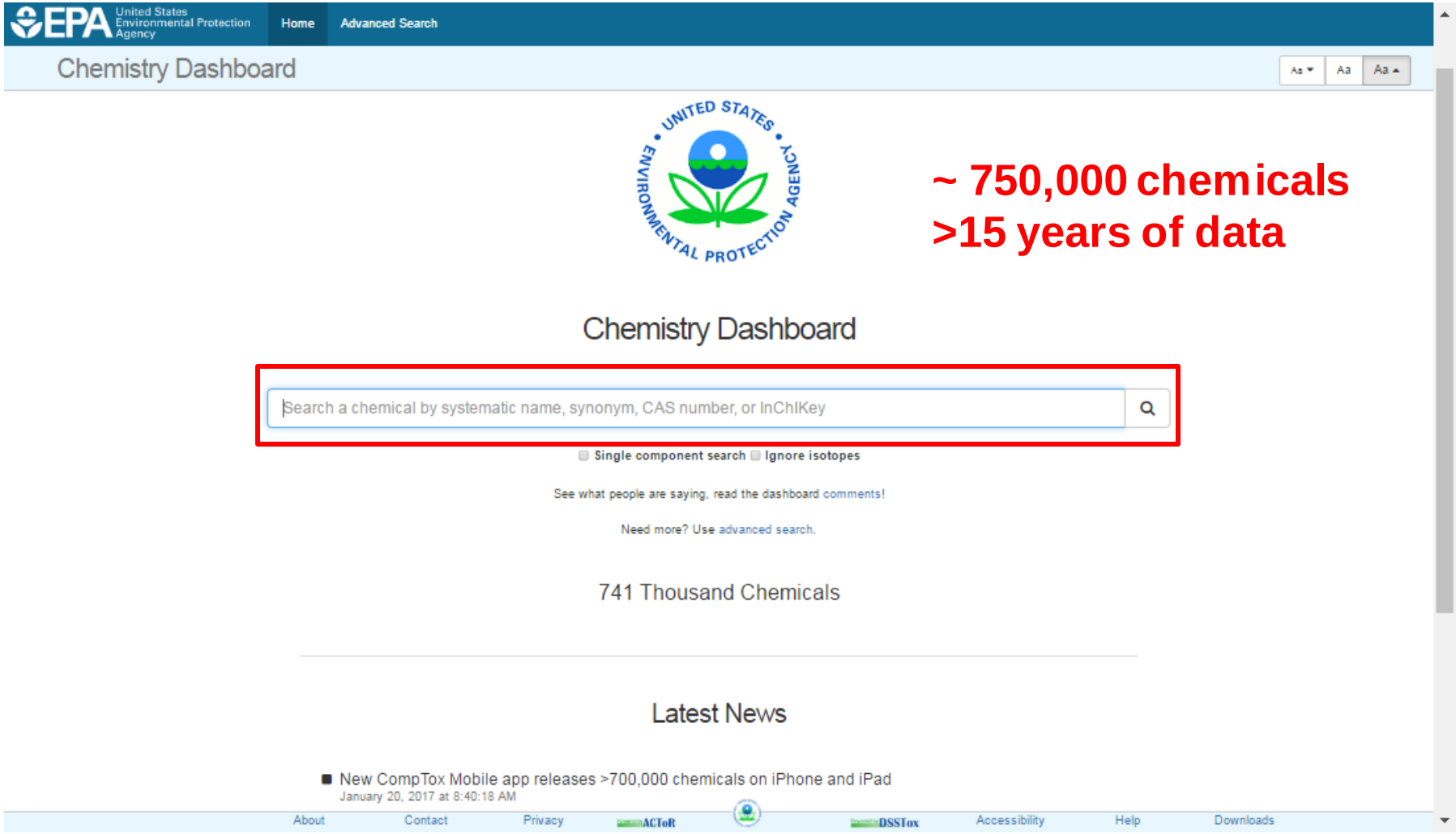

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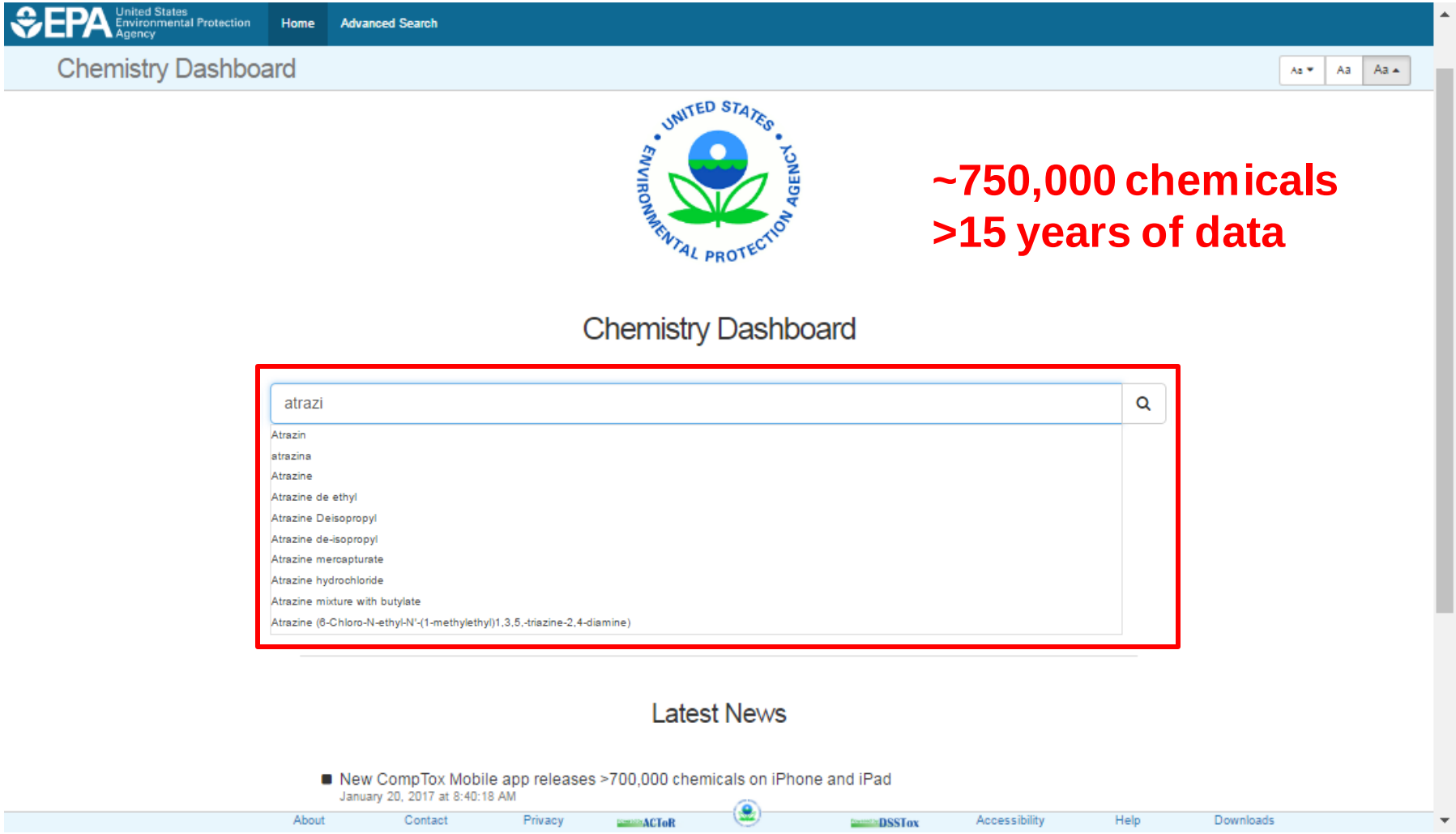


Chemical Page

United States Environmental Protection Agency

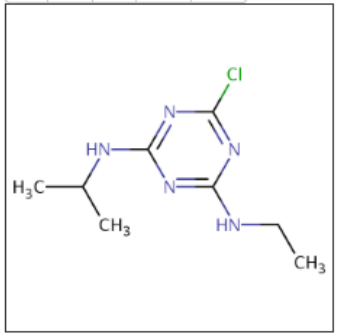
Chemistry Dashboard

Submit Comment | Share | Copy | Aa | Aa | Aa

Atrazine

1912-24-9 | DTXSID9020112

Searched by Approved Name: Found 1 result for 'atrazine'.



Wikipedia

Atrazine is an herbicide of the triazine class. Atrazine is used to prevent pre- and postemergence broadleaf weeds in crops such as maize (corn) and sugarcane and on turf, such as golf courses and residential lawns. It is one of the most widely used herbicides in US and Australian agriculture. It was banned in the European Union in 2004, when the EU found groundwater levels exceeding the limits set by regulators, and Syngenta could neither show that this could be prevented nor that these… Read more

Intrinsic Properties

Structural Identifiers

Related Compounds (Beta)

Presence in Lists

Record Information

Chemical Properties | Env. Fate/Transport | Synonyms | External Links | Toxicity Values (Beta) | Exposure | Bioassays | Similar Molecules (Beta) | Literature | Comments

Chemical Page

United States Environmental Protection Agency

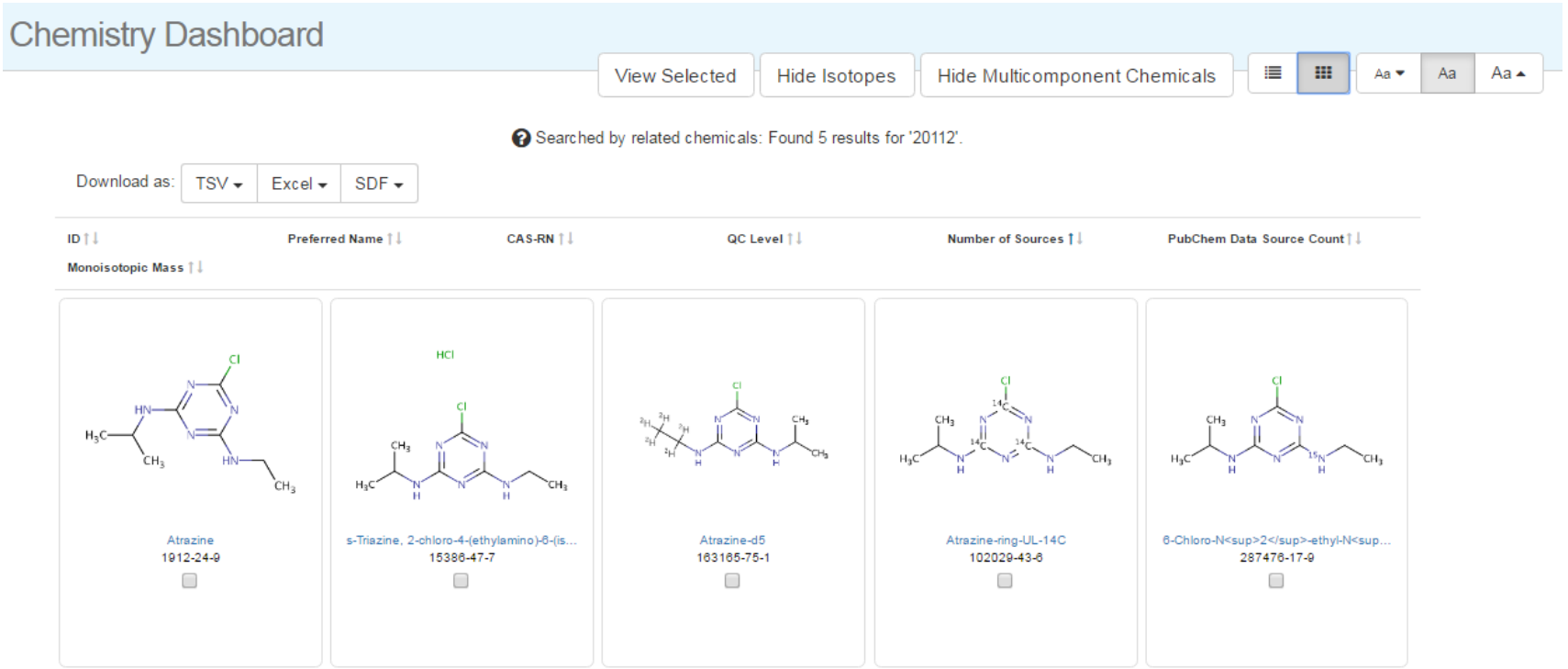
Related Compounds (Beta)

Same Connectivity: 4 records (based on first layer of InChI)

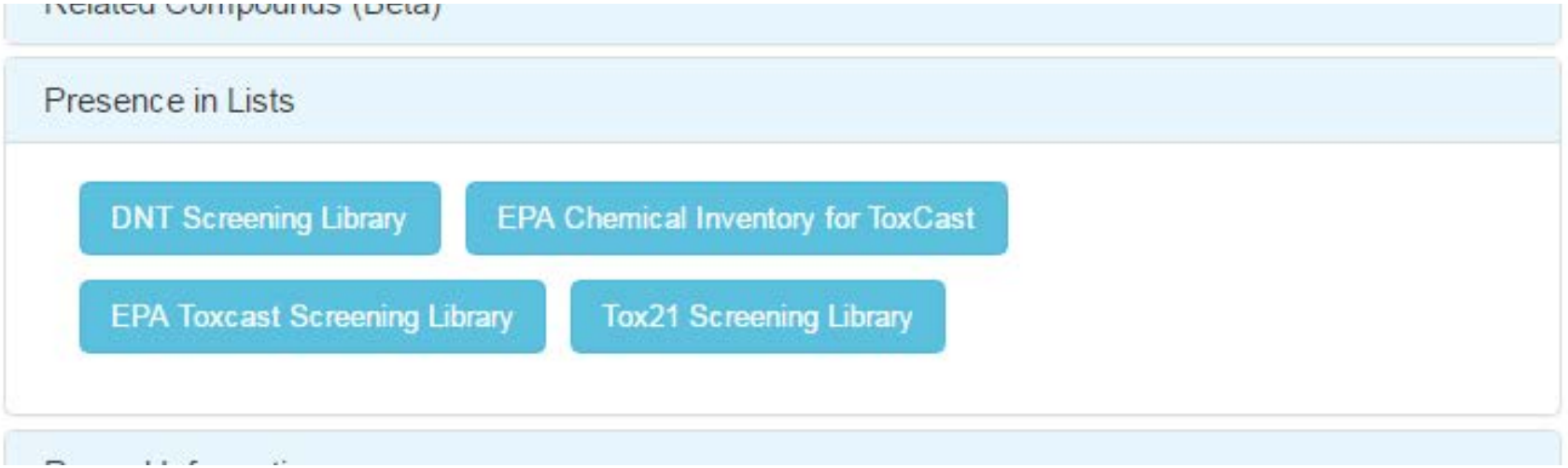
Mixtures, Components, and Neutralized Forms: 5 records (based on QSAR ready mappings and with the compound as a component of a mixture)

Similar Compounds: 62 records (based on Tanimoto coefficient > 0.8)

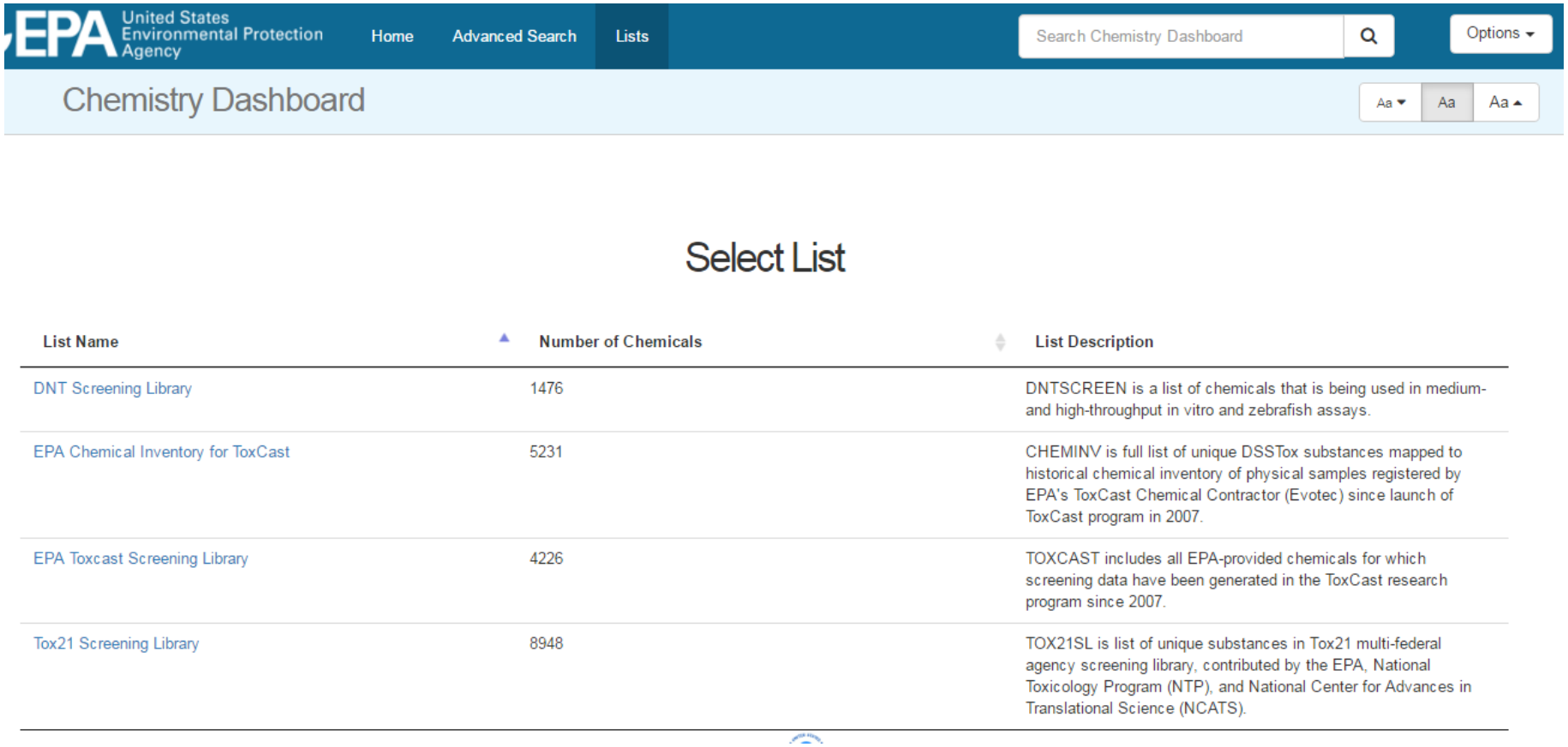
Related Chemicals



Chemical Page
“Is this a ToxCast Chemical?”



Chemical Page
"What are ToxCast Chemicals?"



Chemical Page
"What are ToxCast Chemicals?"

EPA Toxcast Screening Library

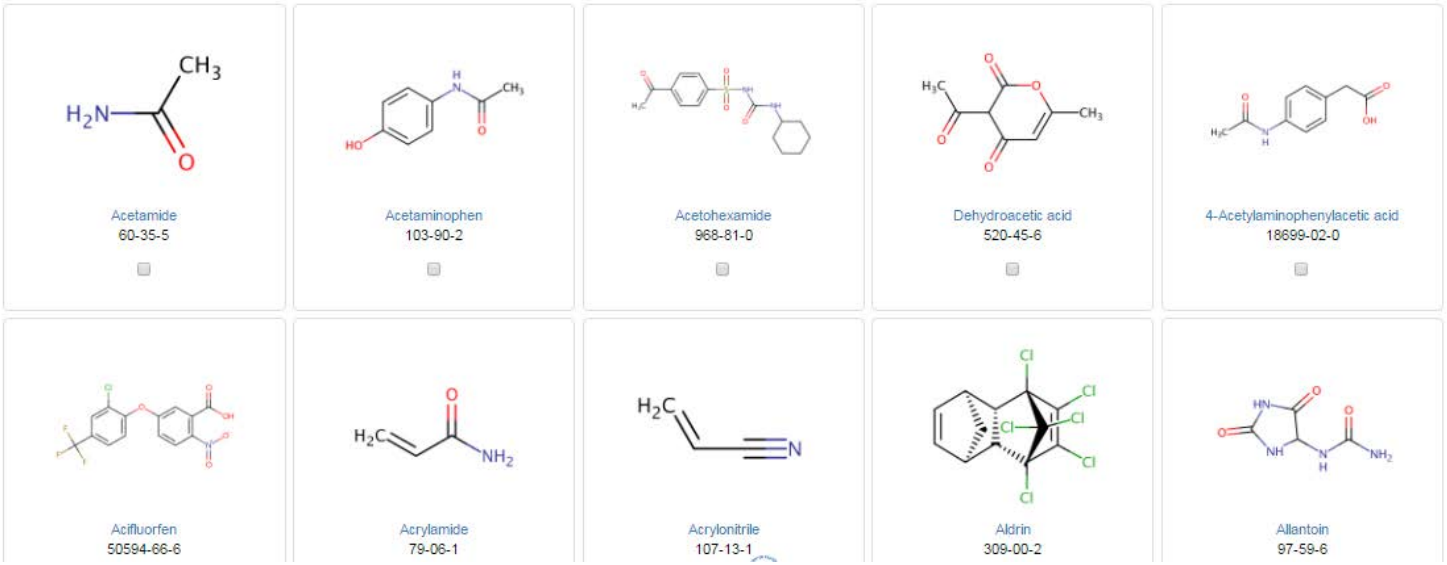
Search TOXCAST Chemicals

List Details

Description: TOXCAST consists of the full list of unique DSSTox substance records (formerly denoted TOXCST) mapped to the historical and present chemical inventory of physical samples plated and screened in the ToxCast program from 2007 to the present. The list includes chemicals that are in current testing, including newly added chemicals as well as discontinued chemicals that have undergone only limited screening. The latter set includes chemicals that were depleted and could not be reprocured (cost, availability), as well as chemicals discontinued for other reasons (e.g., limited solubility, instability, volatility, stench). The TOXCAST inventory also includes EPA's full, plated contribution of nearly 4000 unique chemicals to the multi-federal agency Tox21 program (TOX21SL). The TOXCAST inventory is a complete subset of the CHEMINV physical sample inventory, with the exception of a small set of chemical samples shipped directly to EPA ToxCast vendors or partners or reference chemicals for which EPA ToxCast vendors or partners provided assay data, both of which are included in TOXCAST but not in CHEMINV. A publication detailing the construction and composition of the ToxCast inventory (Richard et al., Chem. Res. Toxicol. 2016), as of January 2016, can be freely downloaded from: http://pubs.acs.org/doi/abs/10.1021/acs.chemrestox.6b00135 For more information on EPA's ToxCast program, see: https://www.epa.gov/chemical-research/toxicity-forecasting To access the ToxCast HTS data within the EPA ToxCast Dashboard, see: https://www.epa.gov/chemical-research/toxcast-dashboard

Number of Chemicals: 4226

Sort Options | Select/Deselect All | **Download as:** TSV | Excel | SDF | View Selected

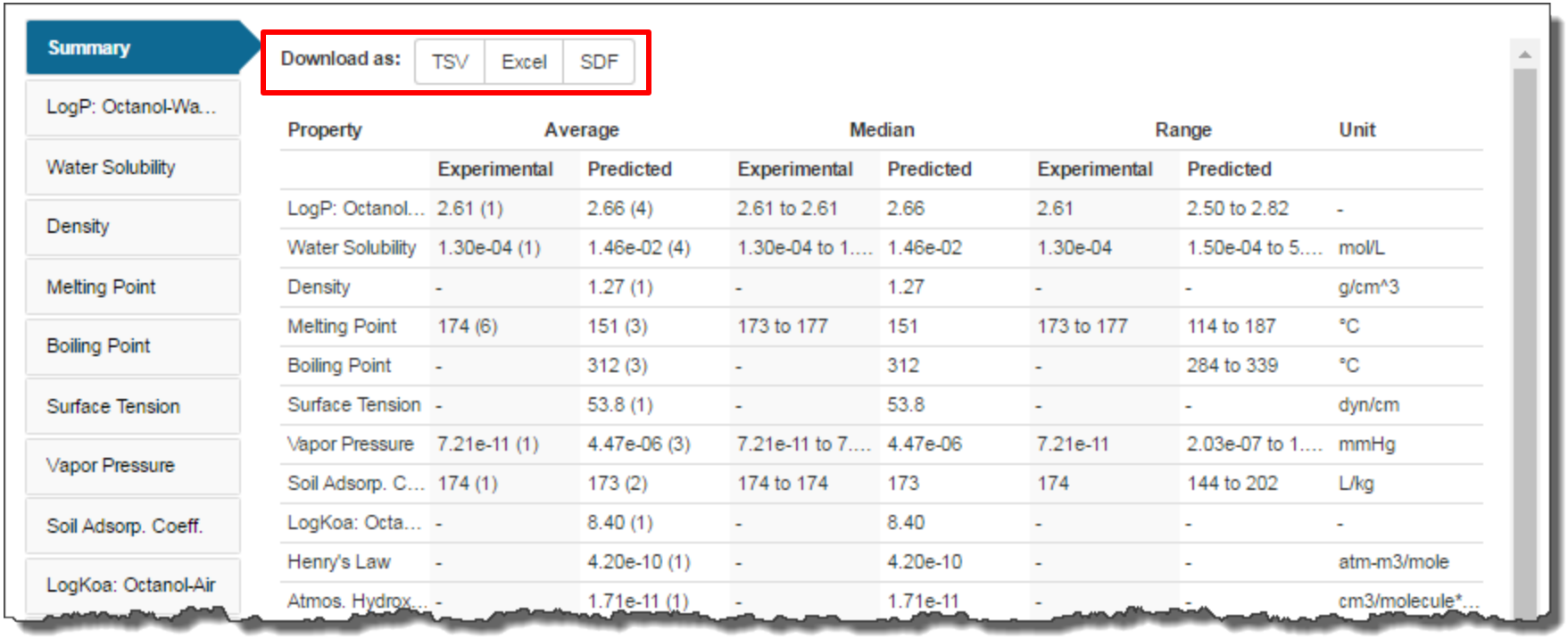


Chemical Page
One button click download..

	A	B	C	D	E	F	G	H	I	J	K	L
1	DTXSID	CAS RN	PREFERRED NAME	IUPAC NAI	MOLECULA	MONOISOT	AVERAGE	SMILES	INCHI KEY			
2	DTXSID905	205939-58-8	Dimethenamid ESA	2-[(1-Metho	C11H17NO5	307.05481	307.38	COCC(C)N(	UZRVVVZNSBSGHK-UHFFFAOYSA-N			
3	DTXSID005	35045-02-4	Metribuzin-DA	6-tert-Butyl-	C8H13N3O5	199.07793	199.27	CSC1=NN=	MIWRSUQXSCLDNV-UHFFFAOYSA-N			
4	DTXSID505	140939-17-9	Alachlor sec-oxanilic acid sodium salt	Sodium (2,6	C12H14NNa	243.08714	243.23801	[Na+].CCC	NQSPCUFTRBYYOS-UHFFFAOYSA-M			
5	DTXSID005	140939-15-7	Alachlor ESA, sodium salt	Sodium 2-[(	C14H20NNa	337.09599	337.37	[Na+].CCC	DXLRATMHMHJKHK-UHFFFAOYSA-M			
6	DTXSID005	64436-13-1	Arsenobetaine	(Trimethylar	C5H11AsO2	177.9975	178.063	C[As+](C)(C	SPTHHTGLGVZZRH-UHFFFAOYSA-N			
7	DTXSID505	52663-68-0	2,2',3,4',5,5',6-Heptachloro-1,1'-biphenyl	2,2',3,4',5,5	C12H3Cl7	391.80544	395.31	ClC1=CC(C	UDMZPLROONOSEF-UHFFFAOYSA-N			
8	DTXSID605	1207-12-1	4,6-Dimethyldibenzothiophene	1,8-Dimethy	C14H12S	212.06597	212.31	CC1=CC2=	KMPJENUWHPZRGZ-UHFFFAOYSA-N			
9	DTXSID705	93-52-7	1,2-dibromo(phenyl)ethane	(1,2-Dibrom	C8H8Br2	261.89928	263.95999	BrCC(Br)C1	SHKKTLSDGJRCTR-UHFFFAOYSA-N			
10	DTXSID805	6174-86-3	3-Chloro-7-hydroxy-4-methyl-2-benzopyrone	3-Chloro-7-h	C10H7ClO3	210.00837	210.61	CC1=C(Cl)C	ODZHLDRQCZXQFQ-UHFFFAOYSA-N			
11	DTXSID505	10482-56-1	(L)-alpha-Terpineol	2-[(1S)-4-M	C10H18O	154.13577	154.25301	CC1=CC[C(	WUOACPNHFRMFPN-SECBINFH			ISA-N
12	DTXSID705	98-02-2	2-Furylmethanethiol	(Furan-2-yl)	C5H6OS	114.01394	114.16	SCC1=CC=	ZFFTZDQKIXPDAF-UHFFFAOYSA-N			
13	DTXSID705	97-89-2	Citronellyl isobutyrate	3,7-Dimethy	C14H26O2	226.19328	226.36	CC(CCOC(=	ZGPPERKMXSGYRK-UHFFFAOYSA-N			
14	DTXSID305	96-54-8	1-Methylpyrrole	1-Methyl-1H	C5H7N	81.057849	81.117996	CN1C=CC=	OXHNLMTVIGZXSG-UHFFFAOYSA-N			
15	DTXSID805	95-56-7	2-Bromophenol	2-Bromophe	C6H5BrO	171.95238	173.009	OC1=C(Br)(	VADKRMSMGWJZCF-UHFFFAOYSA-N			
16	DTXSID005	93-53-8	Hydratropaldehyde	2-Phenylpro	C9H10O	134.07316	134.178	CC(C=O)C1	IQVAERDLDAZARL-UHFFFAOYSA-N			
17	DTXSID005	93-16-3	4-Prop-1-enylveratrole	1,2-Dimetho	C11H14O2	178.09938	178.231	COC1=C(O	NNWHUJCUHAELCL-UHFFFAOYSA-N			
18	DTXSID505	93-02-7	2,5-Dimethoxybenzaldehyde	2,5-Dimetho	C9H10O3	166.06299	166.17599	COC1=CC=	AFUKNJHPZAVHGQ-UHFFFAOYSA-N			
19	DTXSID605	92-91-1	4'-Acetylbiphenyl	1-([1,1'-Biph	C14H12O	196.08882	196.24899	CC(=O)C1=	QCZZSANNLWPGEA-UHFFFAOYSA-N			
20	DTXSID105	91-67-8	N,N-Diethyl-m-toluidine	N,N-Diethyl	C11H17N	163.1361	163.26401	CCN(CC)C1	CIPVVROJHKLHJI-UHFFFAOYSA-N			
21	DTXSID205	91-10-1	2,6-Dimethoxyphenol	2,6-Dimetho	C8H10O3	154.06299	154.16499	COC1=CC=	KUDCXVFHGNTTM-UHFFFAOYSA-N			

Physicochemical Properties

United States Environmental Protection Agency



Summary

LogP: Octanol-Wa...

Water Solubility

Density

Melting Point

Boiling Point

Surface Tension

Vapor Pressure

Soil Adsorp. Coeff.

LogKoa: Octanol-Air

Download as: TSV | Excel | SDF

Property	Average		Median		Range		Unit
	Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
LogP: Octanol...	2.61 (1)	2.66 (4)	2.61 to 2.61	2.66	2.61	2.50 to 2.82	-
Water Solubility	1.30e-04 (1)	1.46e-02 (4)	1.30e-04 to 1....	1.46e-02	1.30e-04	1.50e-04 to 5....	mol/L
Density	-	1.27 (1)	-	1.27	-	-	g/cm^3
Melting Point	174 (6)	151 (3)	173 to 177	151	173 to 177	114 to 187	°C
Boiling Point	-	312 (3)	-	312	-	284 to 339	°C
Surface Tension	-	53.8 (1)	-	53.8	-	-	dyn/cm
Vapor Pressure	7.21e-11 (1)	4.47e-06 (3)	7.21e-11 to 7....	4.47e-06	7.21e-11	2.03e-07 to 1....	mmHg
Soil Adsorp. C...	174 (1)	173 (2)	174 to 174	173	174	144 to 202	L/kg
LogKoa: Octa...	-	8.40 (1)	-	8.40	-	-	-
Henry's Law	-	4.20e-10 (1)	-	4.20e-10	-	-	atm-m3/mole
Atmos. Hydrox...	-	1.71e-11 (1)	-	1.71e-11	-	-	cm3/molecule*...

Physicochemical Properties

United States Environmental Protection Agency

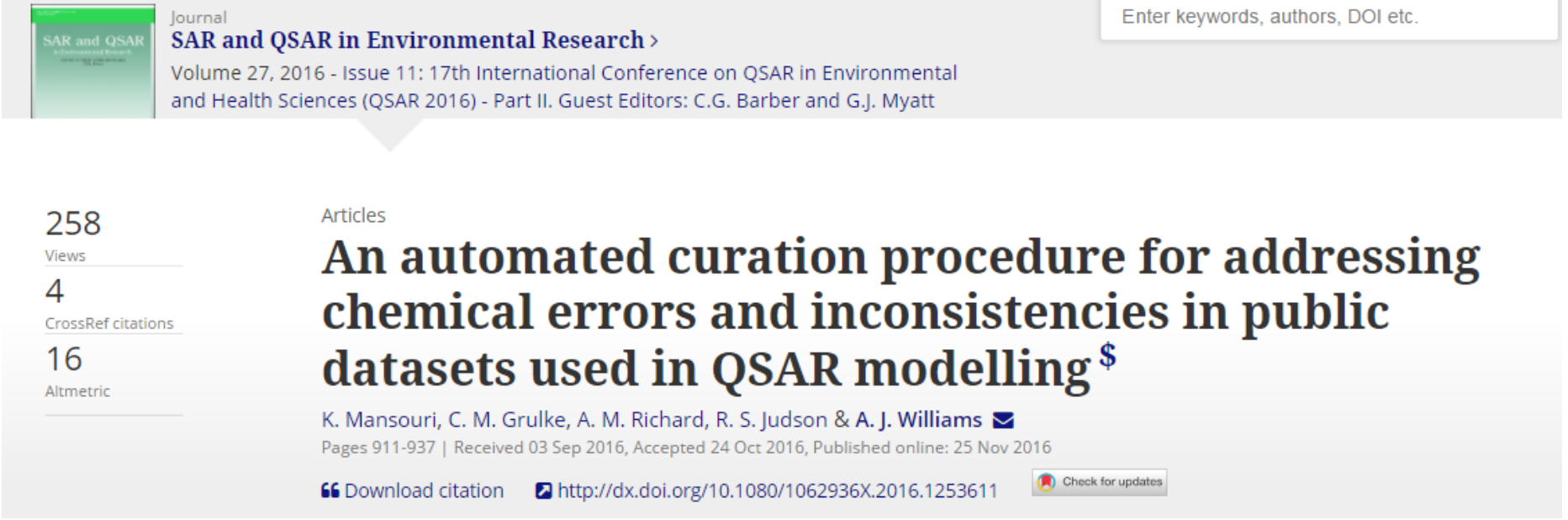
Experimental

Source	Result
PhysPropNCCT	2.61

Predicted

Source	Result	Calculation Details	QMRF
EPISUITE	2.82	Not Available	Not Available
OPERA	3.05	OPERA Model Report	Available
NICEATM	2.50	Not Available	Available
ACD/Labs	2.67	Not Available	Not Available

Workflow Details and Data



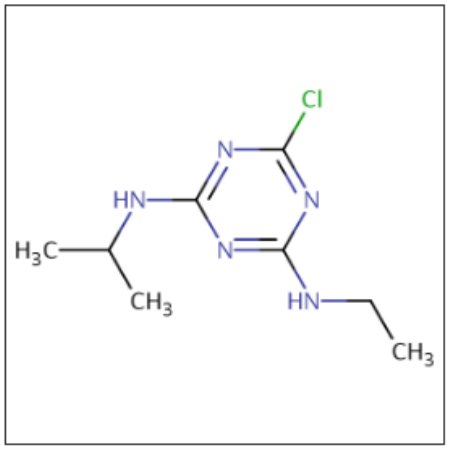
OPERA Models: https://github.com/kmansouri/OPERA

Physicochemical Properties

EPA United States Environmental Protection Agency

Atrazine

1912-24-9 | DTXSID9020112



Model Results

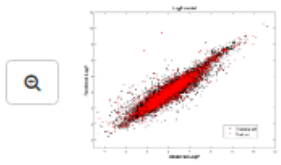
Predicted value: 3.05

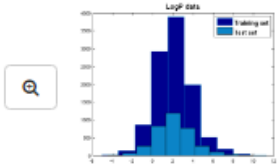
Global applicability domain: Inside

Local applicability domain index: 0.56

Confidence level: 0.77

Model Performance





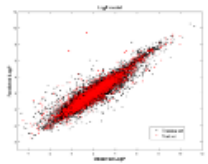
Weighted KNN model

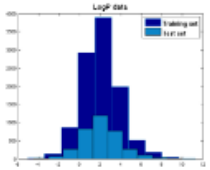
QMRF

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Physicochemical Properties

Model Performance





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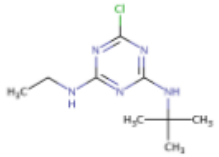
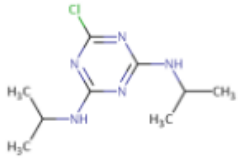
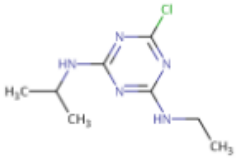
Nearest Neighbors from the Training Set



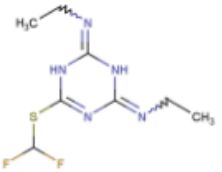
Terbuthylazine
Measured: 3.21
Predicted: 3.74



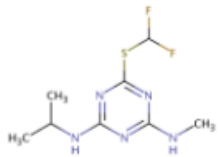
Propazine
Measured: 2.93
Predicted: 3.57



Atrazine
Measured: 2.61
Predicted: 3.05



1,3,5-Triazine,2-difluoromethio-4,6-...
Measured: 3.28
Predicted: N/A



1,3,5-Triazine-2,4-diamine, 6-((diflu...
Measured: 3.27
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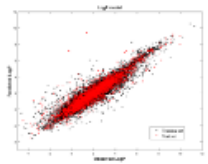
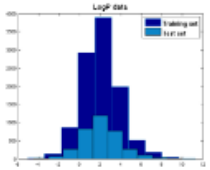
Physicochemical Properties

United States Environmental Protection Agency

Model Performance





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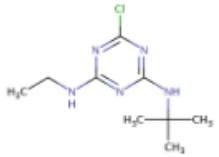

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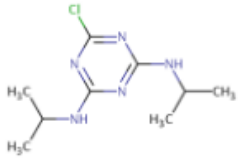

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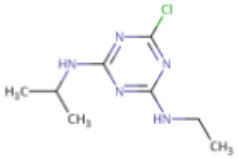

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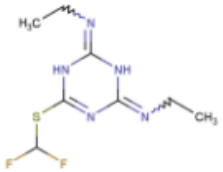
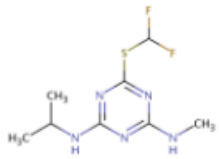
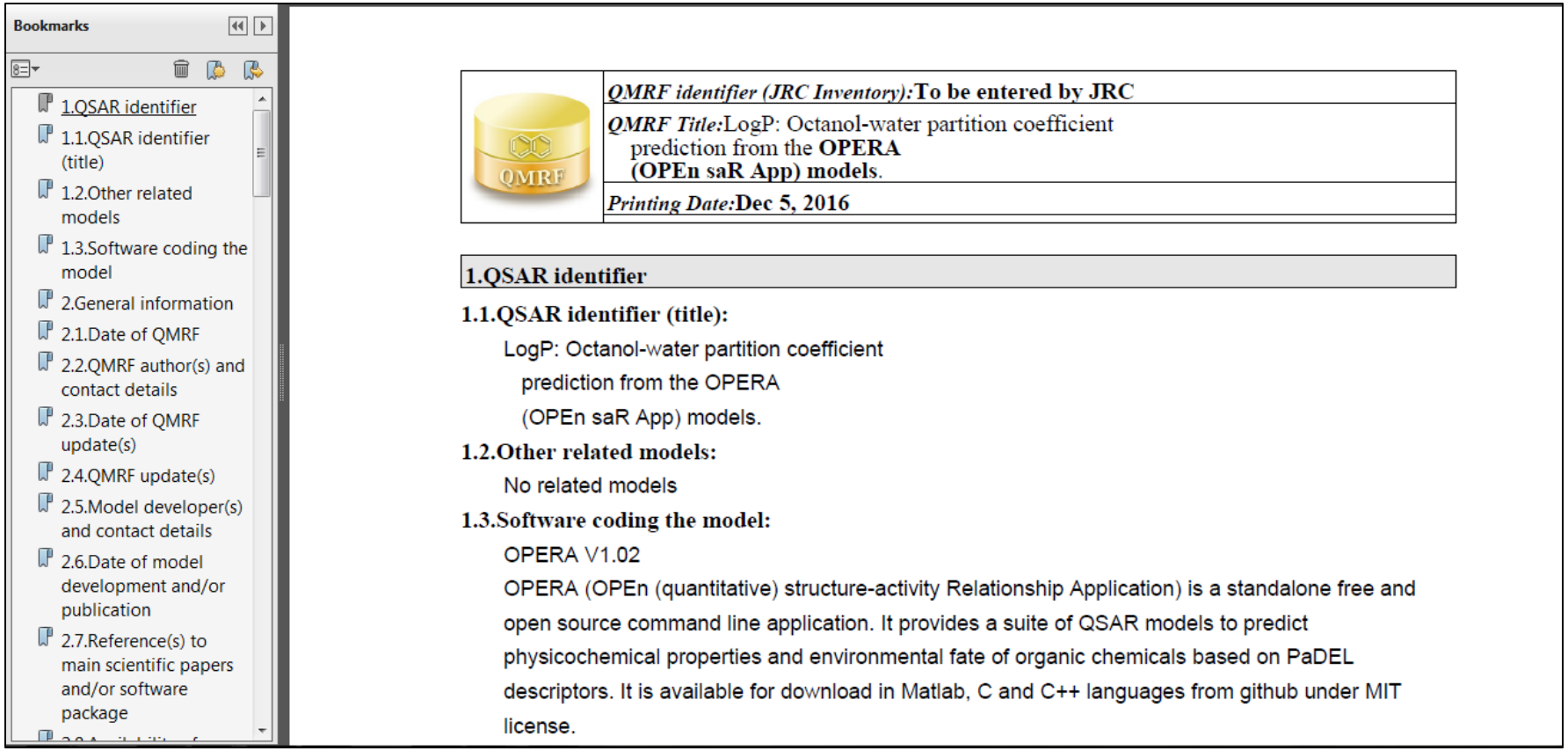


1,3,5-Triazine,2-difluoromethio-4,6-...
Measured: 3.28
Predicted: N/A

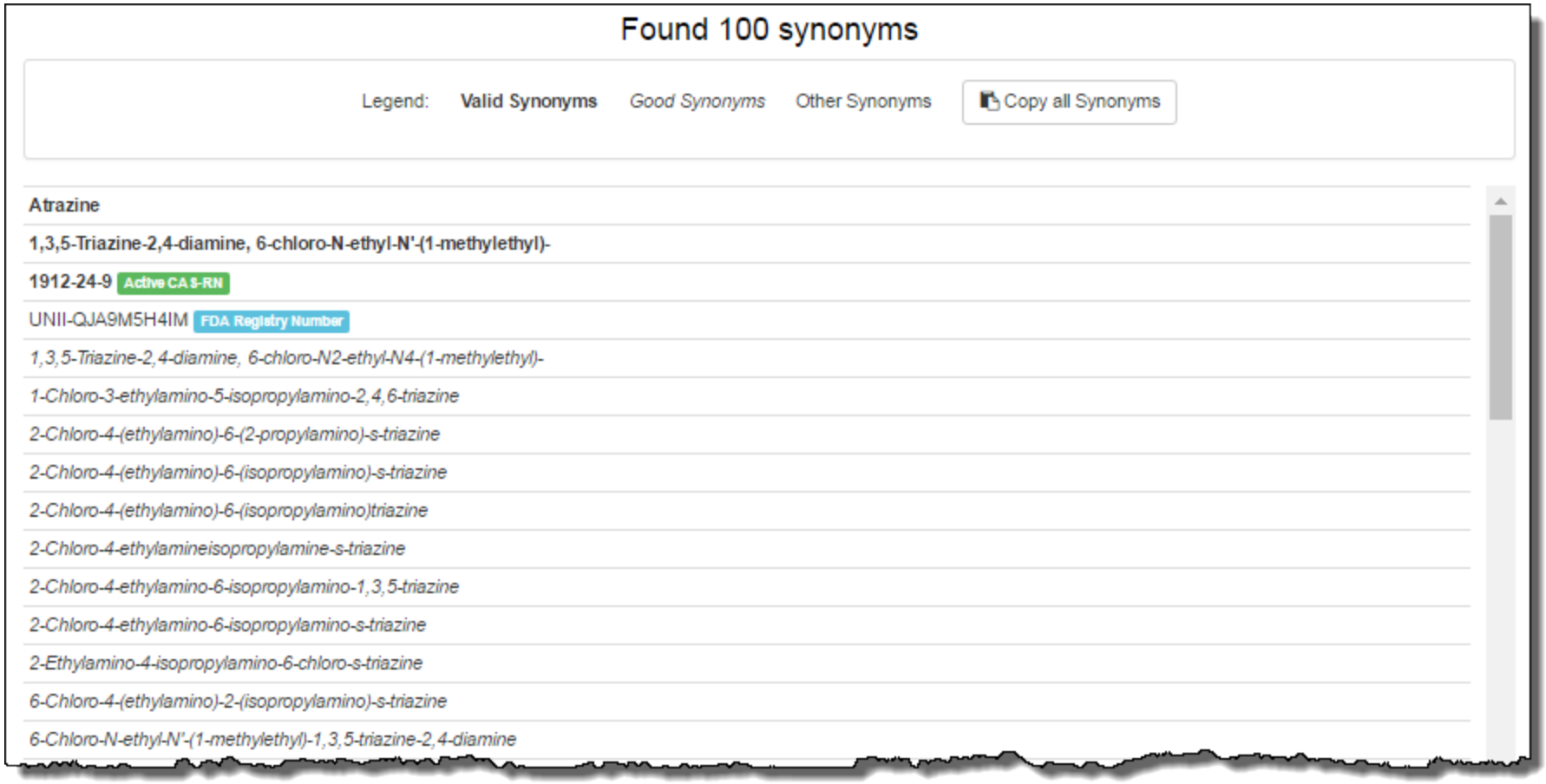


1,3,5-Triazine-2,4-diamine, 6-((diflu...
Measured: 3.27
Predicted: 3.78

Physicochemical Properties



Names and Identifiers



Links to Other Resources

General	Toxicology	Publications	Analytical
EPA Substance Re...	ACToR	Toxline	National Environme...
NIST Chemistry W...	DrugPortal	Environmental Heal...	MONA: MassBank ...
Household Product...	CCRIS	NIEHS	Tox21 Analytical Data
PubChem	ChemView	National Toxicology...	RSC Analytical Abs...
Chemspider	CTD	Google Books	FOR-IDENT
CPCat			
DrugBank			
HMDB			
Wikipedia	HSDB	Federal Register	
MSDS Lookup	ToxCast Dashboar...	Regulations.gov	
ChEMBL	LactMed	Springer Materials	
Chemical Vendors	ACToR PDF Report	BioCaddie DataMed	
Consumer Product...	International Toxicit...	RSC Publications	

The Office of the Federal Register (OFR) of the National Archives and Records Administration (NARA), and the U.S. Government Printing Office (GPO) jointly administer the FederalRegister.gov website.

Exposure

United States Environmental Protection Agency

- Chemical Weight F...
- Product Use Categ...
- Chemical Function...
- Monitoring Data
- Exposure Predictions

Chemical Weight Fractions

Download as: TSV | Excel

Product Name	Specific/ Generic	Product Use Category	Reported Functional Use	Minimum Weight Fraction	Maximum Weight Fraction	Data Type
bonus s max + fire..	Specific	pesticides: insecti...	-	0.0	0.01069	MSDS
bonus s max 10m 1	Specific	landscape/yard: la..	-	0.0	0.01089	MSDS
bonus s max 5m 1	Specific	landscape/yard: la..	-	-	-	MSDS
expert gardener s...	Specific	landscape/yard: g...	-	0.0125	0.0125	MSDS
expert gardener s...	Specific	landscape/yard: g...	-	0.0125	0.0125	MSDS
scotts bonus s ma...	Specific	pesticides: insecti...	-	-	-	MSDS
scotts bonus s 29...	Specific	landscape/yard: la..	-	0.0111	0.0111	MSDS
scotts bonus s ma...	Specific	pesticides: insecti...	-	0.01352	0.01352	MSDS
scotts bonus s, 53...	Specific	landscape/yard: la..	-	0.01293	0.01293	MSDS
spectracide weed...	Specific	landscape/yard: h...	-	0.04	0.04	MSDS

Exposure

United States Environmental Protection Agency

- Chemical Weight F...
- **Product Use Cate...**
- Chemical Function...
- Monitoring Data
- Exposure Predictions

Product Use Categories (PUCs)

Download as: TSV | Excel

Product Use Category	Product Name	Source	Product Date
pesticides: insecticide	bonus s max + fireant killer 12m 1	Retail Product Categories/Walmart	-
landscape/yard: lawn fertilizer	bonus s max 10m 1	Retail Product Categories/Walmart	-
landscape/yard: lawn fertilizer	bonus s max 5m 1	Retail Product Categories/Walmart	-
landscape/yard: garden fertilizer	expert gardener st augustine wee...	Retail Product Categories/Walmart	2006-06-22
landscape/yard: garden fertilizer	expert gardener st. augustine we...	Retail Product Categories/Walmart	-
pesticides: insecticide	scotts bonus s max with fire ant ki...	Retail Product Categories/Walmart	-
landscape/yard: lawn fertilizer	scotts bonus s 29-3-4 1	Retail Product Categories/Walmart	-
pesticides: insecticide	scotts bonus s max w/fireant klr, 5...	Retail Product Categories/Walmart	-
landscape/yard: lawn fertilizer	scotts bonus s, 538-18 1	Retail Product Categories/Walmart	-
landscape/yard: herbicide	spectracide weed stop concentrat...	Retail Product Categories/Walmart	-

Exposure

United States Environmental Protection Agency

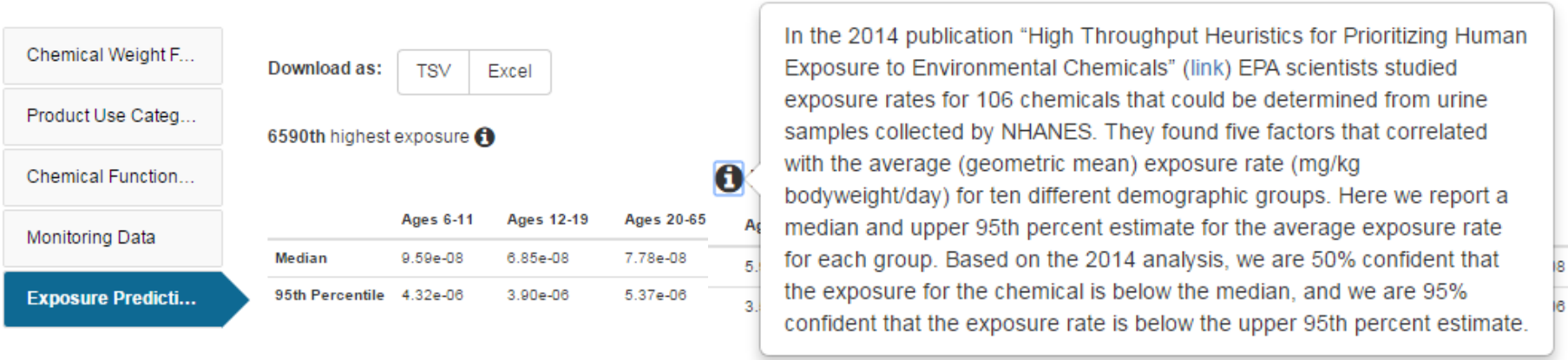
- Chemical Weight F...
- Product Use Categ...
- Chemical Function...
- **Monitoring Data**
- Exposure Predictions

Download as: TSV | Excel

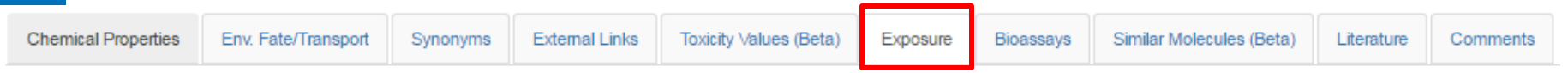
National Health and Nutrition Examination Survey (NHANES) Inferences (mg/kg-bw/day)

	Ages 6-11	Ages 12-19	Ages 20-65	Ages 65+	BMI > 30	BMI < 30	Repro. Age Females	Females	Males	Total
Lower 95th Limit	3.21e-09	1.84e-09	5.53e-09	2.42e-09	3.56e-09	3.70e-09	3.96e-09	4.30e-09	1.71e-09	2.81e-09
Upper 95th Limit	4.23e-07	4.70e-07	4.38e-07	4.97e-07	4.01e-07	4.63e-07	5.39e-07	4.34e-07	3.75e-07	3.81e-07
Median	4.79e-08	5.21e-08	7.79e-08	6.93e-08	6.19e-08	5.98e-08	8.17e-08	7.04e-08	4.20e-08	5.76e-08

Exposure



- *Navigation aids, including these hovers, are being added to make navigation and understanding easier. Movies are in development.*



In vitro Bioassay Data

- *In vitro* **bioassays** are used to determine the biological activity of a substance – **Toxcast project**
- A decade of measurements, and millions of dollars of data integrated into the dashboard

NVS_GPCR_hAdoRA1

Assay Name: NVS_GPCR_hAdoRA1

Gene Symbol: ADORA1

Organism: human

Tissue: brain

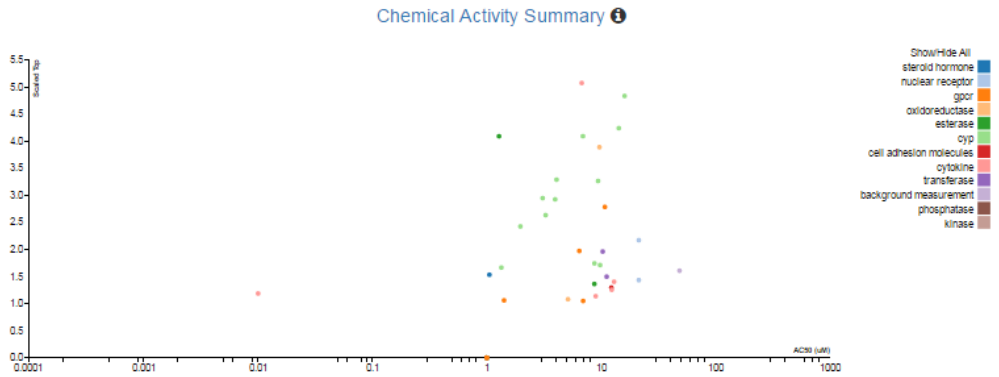
Assay Format Type: biochemical

Biological Process Target: receptor binding

Detection Technology: Radiometry

Analysis Direction: positive

Intended Target Family: gpcr



Download as: TSV | Excel | Show Inactive | Show Background Result

Assay Name	Hit Call	Top	Scaled Top	AC50	log AC50	Intended Target Family
CEETOX_H295R_ESTRONE_up	ACTIVE	1.24	1.53	1.06	0.0236	steroid hormone

Chemical Properties | Env. Fate/Transport | Synonyms | External Links | Toxicity Values (Beta) | Exposure | Bioassays | Similar Molecules (Beta) | Literature | Comments

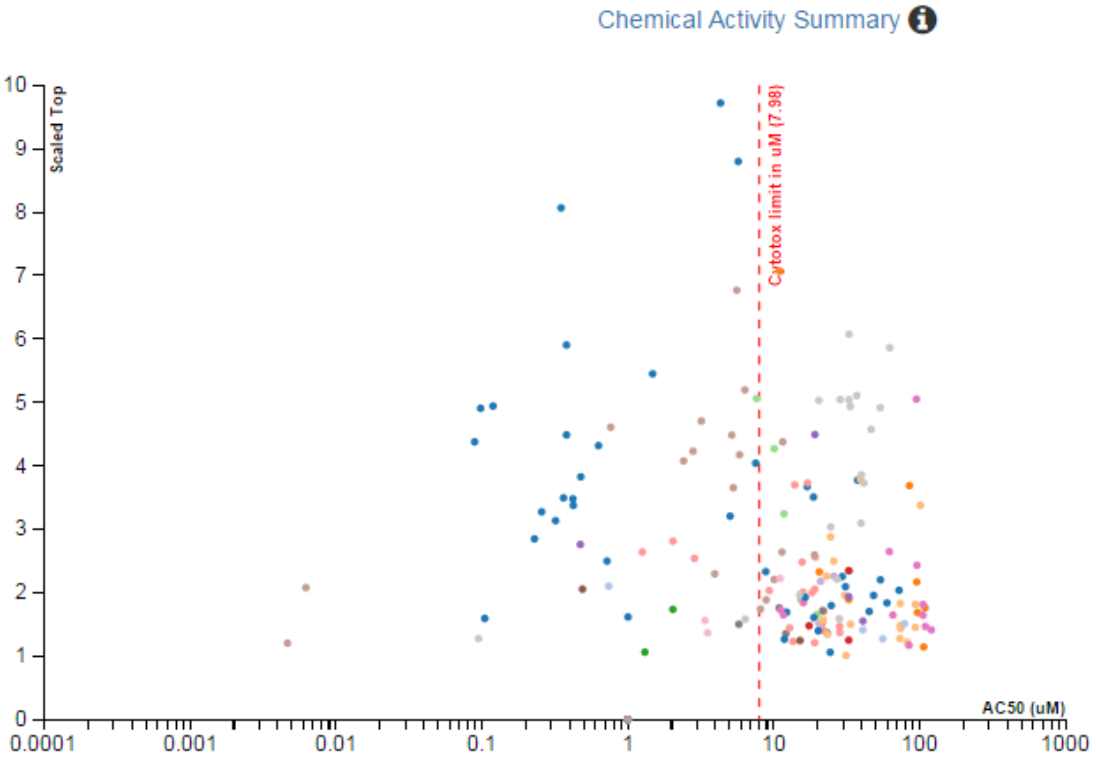
ToxCast and Tox21 Bioassays

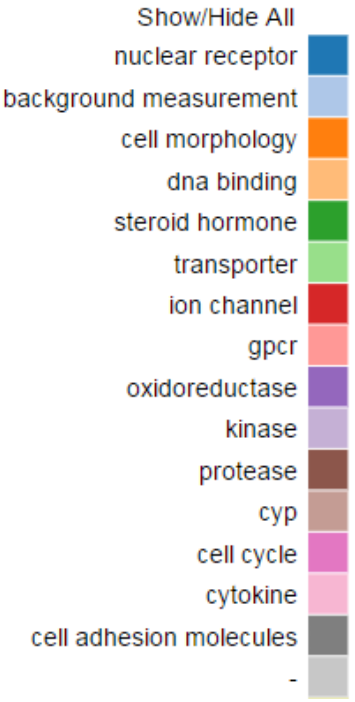
United States Environmental Protection Agency

ToxCast

PubChem

ScrubChem (Beta)





Chemical Properties | Env. Fate/Transport | Synonyms | External Links | Toxicity Values (Beta) | Exposure | Bioassays | Similar Molecules (Beta) | Literature | Comments

ToxCast and Tox21 Bioassays

United States Environmental Protection Agency

Download as: TSV | Excel Show: Inactive | Background

Assay Name	Hit Call	Top	Scaled Top	AC50	log AC50 ↓	Intended Target Family
APR_Hepat_CellLoss_48hr_dn	ACTIVE	1.41	1.41	120	2.08	cell cycle
APR_HepG2_MitoMass_24h_dn	ACTIVE	0.874	1.76	109	2.04	cell morphology
APR_HepG2_OxidativeStress_24h_up	ACTIVE	1.20	1.47	110	2.04	cell cycle
APR_Hepat_DNADamage_48hr_up	ACTIVE	1.84	1.14	107	2.03	cell morphology
APR_HepG2_CellLoss_24h_dn	ACTIVE	1.20	1.81	106	2.02	cell cycle
APR_HepG2_OxidativeStress_72h_up	ACTIVE	1.80	1.65	106	2.02	cell cycle
ATG_HSE_CIS_up	ACTIVE	1.59	3.38	102	2.01	dna binding

PubChem Bioassay Data Integration

United States Environmental Protection Agency

ToxCast

PubChem

ScrubChem (Beta)

PubChem Biological Activities

PUBCHEM > COMPOUND > BISPHENOL A > BIOLOGICAL TEST RESULTS > BIOASSAY RESULTS >

BioAssay Results

Refine/Analyze Download

All (1,852) | Active(92) | Inconclusive(135) | Inactive(1,038) | Unspecified(587)

1 to 10 of 92 1 2 3 ... 10 Activity

Activity	Activity Value [µM]	Substance SID	BioAssay AID	BioAssay Name	Target
Active		81140	155	NCI Yeast Anticancer Drug Screen. Data for the rad50 strain	
Active		81140	157	NCI Yeast Anticancer Drug Screen. Data for the mec2-1 strain	
Active		68531	161	NCI Yeast Anticancer Drug Screen. Data for the sgs1 mgt1 strain	
Active		81140	165	NCI Yeast Anticancer Drug Screen. Data for the cln2 rad14 strain	
Active		81140	167	NCI Yeast Anticancer Drug Screen. Data for the bub3 strain	

Chemical Properties | Env. Fate/Transport | Synonyms | External Links | Toxicity Values (Beta) | Exposure | Bioassays | Similar Molecules (Beta) | Literature | Comments

Integrated Literature Searching

EPA United States Environmental Protection Agency

PubChem

BioAssay | Compound | Substance

Google Scholar

atrazine

PubMed

PubMed comprises more than 26 million citations for biomedical literature from MEDLINE, life science journals, and online books. Citations may include links to full-text content from PubMed Central and publisher web sites.

Chemical Properties | Env. Fate/Transport | Synonyms | External Links | Toxicity Values (Beta) | Exposure | Bioassays | Similar Molecules (Beta) | Literature | Comments

Integrated Literature Searching

United States Environmental Protection Agency

PubChem Artic...
Google Scholar
Abstract Sifter
PubChem Patents

PubChem Articles

PUBCHEM > COMPOUND > ATRAZINE > LITERATURE > DEPOSITOR PROVIDED PUBMED CITATIONS >

Depositor Provided PubMed Citations

Download

1 to 10 of 876 1 2 3 ... 88 Date

PMID	Date	Title	Journal
26923738	2016-06-01	Atrazine blocks ovulation via suppression of Lhr and Cyp19a1 mRNA and estradiol secretion in immature gonadotropin-treated rats.	Reproductive toxicology (Elmsford, N.Y.)
27114639	2016-03-01	Atrazine exposure causes mitochondrial toxicity in liver and muscle cell lines.	Indian journal of pharmacology
26647222	2016-01-05	Endocrine-Disrupting Effects of Pesticides through Interference with Human Glucocorticoid Receptor.	Environmental science & technology
26464060	2016-01-01	Effects of Neonicotinoids on Promoter-Specific Expression and Activity of Aromatase (CYP19) in Human Adrenocortical Carcinoma (H295R) and Primary Umbilical Vein Endothelial (HUVEC) Cells.	Toxicological sciences : an official journal of the Society of Toxicology
26377646	2015-09-16	Atrazine-Mediated Disruption of Steroidogenesis in BLTK1 Murine Leydig Cells.	Toxicological sciences : an official journal of the Society of Toxicology

Chemical Properties | Env. Fate/Transport | Synonyms | External Links | Toxicity Values (Beta) | Exposure | Bioassays | Similar Molecules (Beta) | Literature | Comments

Integrated Literature Searching

United States Environmental Protection Agency

PubChem Articles

Google Scholar

Abstract Sifter

PubChem Patents

Select Term: Environmental AND Non-targeted Analysis AND -

Edit the Query Before Querying (73 Characters)

"Non-targeted Analysis" AND "Environmental" AND "1912-24-9" OR "Atrazine"

Submit

Chemical Properties | Env. Fate/Transport | Synonyms | External Links | Toxicity Values (Beta) | Exposure | Bioassays | Similar Molecules (Beta) | Literature | Comments

Integrated Literature Searching

United States Environmental Protection Agency

PubChem Articles

Google Scholar

Abstract Sifter

PubChem Patents

Select Term: Environmental AND Non-targeted Analysis AND -

Edit the Query Before Querying (73 Characters)

"Non-targeted Analysis" AND "Environmental" AND "1912-24-9" OR "Atrazine"

Google "Non-targeted Analysis" AND "Environmental" AND "1912-24-9" OR "Atrazir

Scholar About 30 results (**0.14** sec) My Citations 10

Articles
Case law
My library

Any time
Since 2017
Since 2016
Since 2013
Custom range...

Sort by relevance
Sort by date

include patents
include citations

Create alert

Environmental metabolomics: a critical review and future perspectives [PDF] academia.edu
JG Bundy, MP Davey, MR Viant - Metabolomics, 2009 - Springer
... Hence, several steps must now to taken to move **environmental** metabolomics forward, as discussed below, including issues related to ... And for a relatively rapid, quantitative and **non-targeted analysis** of the most abundant metabolites one could select the well-established ...
Cited by 306 Related articles All 9 versions Cite Save

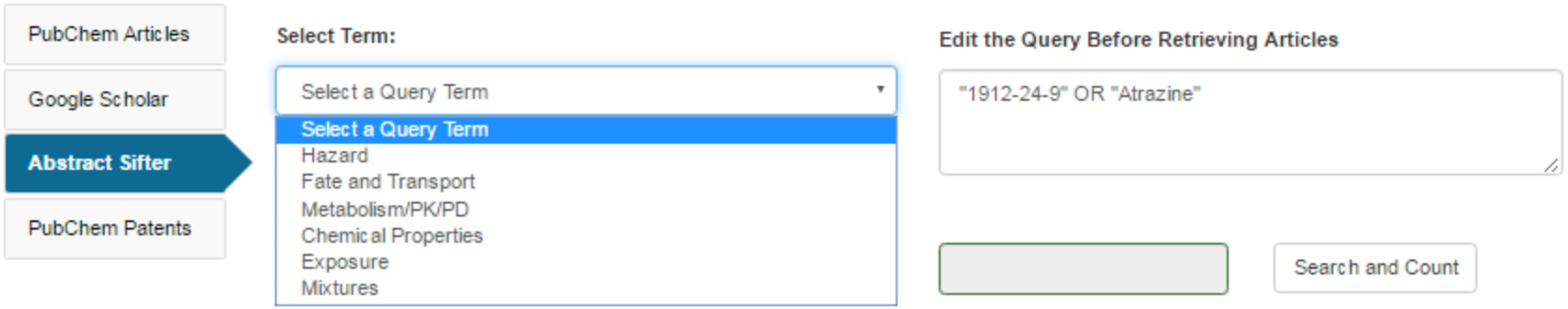
New trends in the analytical determination of emerging contaminants and their transformation products in **environmental** waters [PDF] researchgate.net
A Agüera, MJM Bueno, AR Fernández-Alba - **Environmental** Science and ..., 2013 - Springer
... Take survey. Download PDF. **Environmental** Science and Pollution Research. **Environmental** Science and Pollution Research. ... New trends in the analytical determination of emerging contaminants and their transformation products in **environmental** waters. ...
Cited by 51 Related articles All 10 versions Cite Save

Coupling passive sampling and time of flight mass spectrometry for a better estimation of polar pesticide freshwater contamination: simultaneous target quantification …
R Guibal, S Lissalde, A Charriau, G Poulier... - ... of Chromatography A, 2015 - Elsevier
... The proposed quantification method was validated for 43 compounds with variation of calibration slopes below 10% in **environmental** matrix. For the unvalidated compound DIA (**atrazine**-desisopropyl: an **atrazine** metabolite), interference increased the error of concentration ...
Cited by 12 Related articles All 5 versions Cite Save

Chemical Properties | Env. Fate/Transport | Synonyms | External Links | Toxicity Values (Beta) | Exposure | Bioassays | Similar Molecules (Beta) | Literature | Comments

Integrated Literature Searching

United States Environmental Protection Agency



Integrated Literature Searching

United States Environmental Protection Agency

PubChem Articles
Google Scholar
Abstract Sifter
PubChem Patents

Select Term:

Hazard

Retrieve Articles | 23 Articles (out of 23)

Edit the Query Before Retrieving Articles

("1912-24-9" OR "Atrazine") AND (NOAEL or LOEL or Rfd OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])

Add additional query terms to filter abstracts:

Search and Count

Term 1	Term 2	Term 3	Total	PMID	PubYr	Title
0	0	0	0	26260...	2015	Using species sensitivity distribution approach to assess the risks ...
0	0	0	0	25138...	2014	Effect of atrazine and fenitrothion at no-observed-effect-levels (NO...
0	0	0	0	24797...	2014	Multigeneration reproduction and male developmental toxicity studi...
0	0	0	0	24323...	2013	Evaluation of hydroxyatrazine in the endocrine disruptor screening ...

Record: 1 of 23

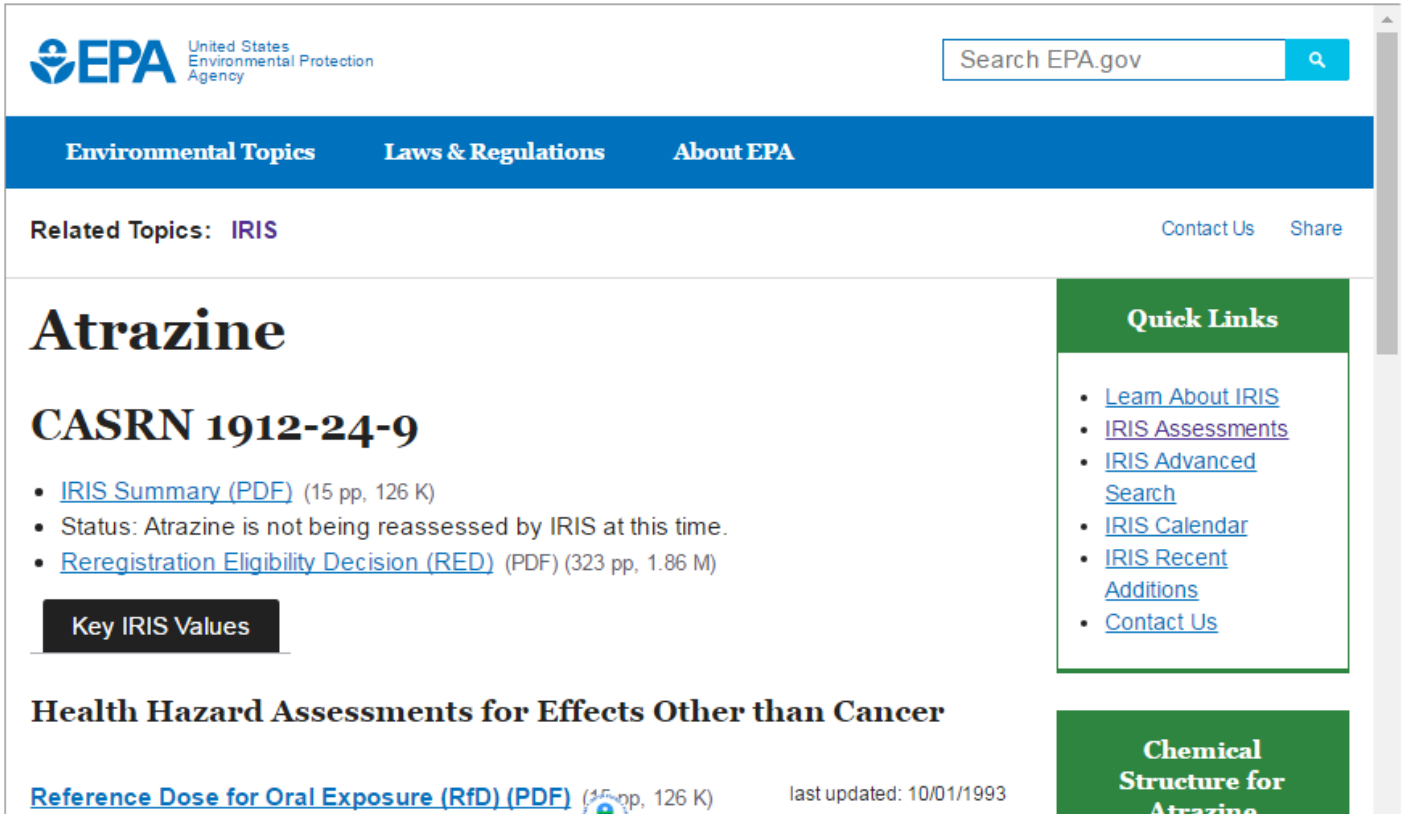
Title: Using species sensitivity distribution approach to assess the risks of commonly detected agricultural pesticides to Australia's tropical freshwater ecosystems.

Abstract: To assess the potential impacts of agricultural pesticides on tropical freshwater ecosystems, the present study developed temperature-specific, freshwater species protection concentrations (i.e., ecotoxicity threshold values) for 8 pesticides commonly detected in Australia's tropical freshwaters. Because relevant toxicity data for native tropical freshwater species to assess the ecological risks were mostly absent, scientifically robust toxicity data obtained at ≥20 °C were used for ecologically relevant taxonomic groups representing primary producers and consumers. Species sensitivity distribution (SSD) curves were subsequently generated for predicted chronic exposure using Burrlioz 2.0 software with mixed chronic and converted acute data relevant to exposure conditions at ≥20 °C. Ecotoxicity threshold values for tropical freshwater ecosystem

Integrated Literature

United States Environmental Protection Agency

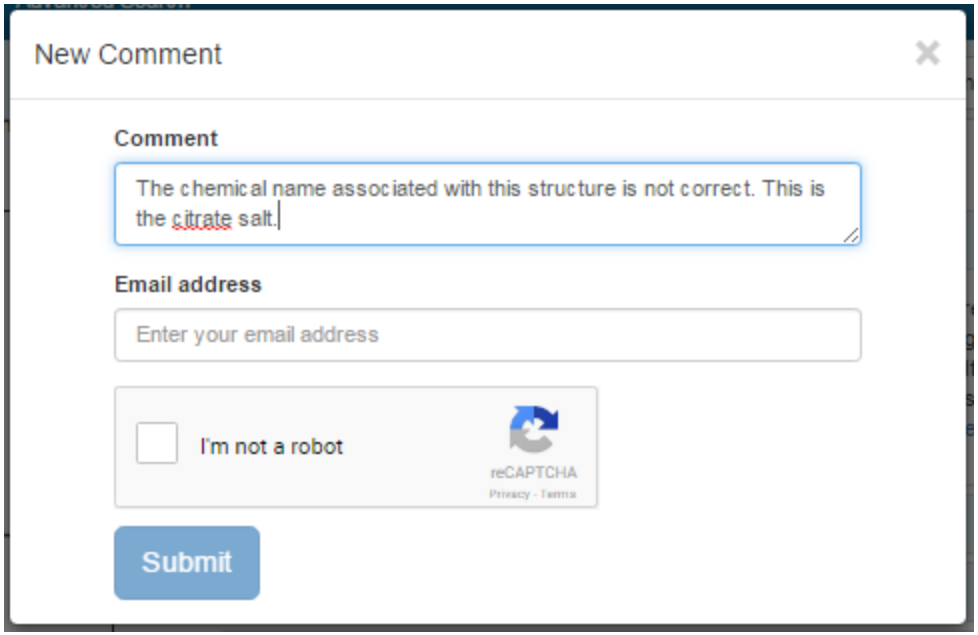
- Google Scholar
- Abstract Sifter
- PubChem Articles
- PubChem Patents
- IRIS



Chemical Properties | Env. Fate/Transport | Synonyms | External Links | Toxicity Values (Beta) | Exposure | Bioassays | Similar Molecules (Beta) | Literature | Comments

Crowdsourced Data Curation

- Maintaining high-quality data is a challenge
- Every user can contribute to improving the data!



Chemical Properties | Env. Fate/Transport | Synonyms | External Links | Toxicity Values (Beta) | Exposure | Bioassays | Similar Molecules (Beta) | Literature | Comments

“UVCBs” - Unknown or Variable Composition, Complex Reaction Products and Biological Materials

C3-C15 Sulfophenyl carboxylates

NOCAS_891722 | DTXSID90891722

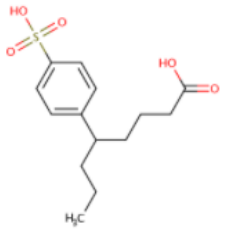
Searched by Approved Name: Found 1 result for 'C3-C15 Sulfophenyl carboxylates'.

Presence in Lists

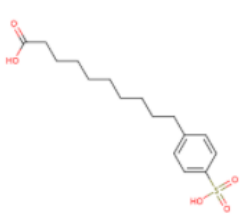
MassBank.EU Collection: Special Cases | Surfactant List Screened in Swiss Wastewater (2014)

Record Information

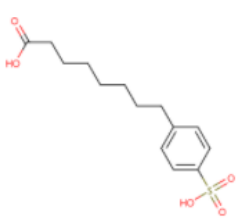
Download as: TSV | Excel | SDF



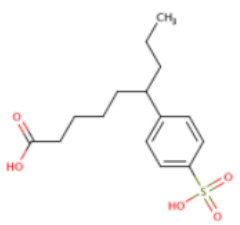
SPA-8C
NOCAS_881094



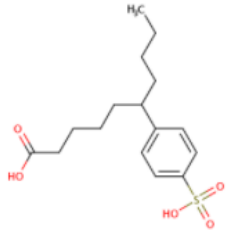
10-(4-sulfophenyl)decanoic acid
NOCAS_891332



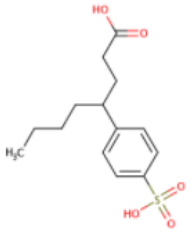
8-(4-sulfophenyl)octanoic acid
NOCAS_891334



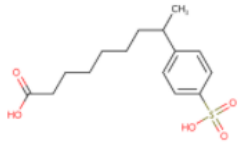
6-(4-sulfophenyl)nonanoic acid
NOCAS_891335



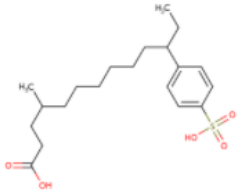
6-(4-sulfophenyl)decanoic acid
NOCAS_891340



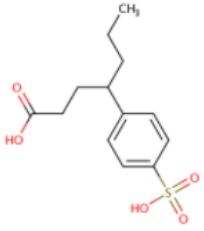
4-(4-sulfophenyl)octanoic acid
NOCAS_891637



8-(4-sulfophenyl)nonanoic acid
NOCAS_891660



4-methyl-11-(4-sulfophenyl)tridecanoic ...
NOCAS_891661



4-(4-sulfophenyl)heptanoic acid
NOCAS_891662

Some Typical Questions

- I have a 1000 CAS Numbers (or Names) – are there data available?
  - Has any Toxcast data been run?
  - Are there Toxicity Data values available?
  - Are there predicted exposure data (via Expocast)?
  - Can I get predicted physchem data for my model?

Batch Searching for Data for Thousands of Chemicals

- What are these chemicals?

Chemicals Used in the Hydraulic Fracturing Process in Pennsylvania
Prepared by the Department of Environmental Protection
Bureau of Oil and Gas Management

Updated June 10, 2010

Chemical	Product Name
2,2-Dibromo-3-Nitrilopropionamide	Bio Clear 1000/Bio Clear 2000/ Bio-Clear 200/BioRid20L/ EC6116A
2-methyl-4-isothiazolin-3-one	X-Cide 207
5-chloro-2-methyl-4-isothiazolin-3-one	X-Cide 207
Acetic Acid	Fe-1A Acidizing Composition/ Packer Inhibitor
Acetic Anhydride	Fe-1A Acidizing Composition
Acetylene	GT&S Inc./ Airco
Alcohol Ethoxylated	C12-16 NE-200
Alkyl benzene sulfonic acid	Tetrolite AW0007/ FR-46
Ammonia (aqueous)	FAW-5
Ammonium Bifluoride	ABF 37%
Ammonium Persulfate	AP Break
Ammonium Bisulfite	Techni-Hib 604/ Fe OXCLEAR/ Packer Inhibitor
Ammonium chloride	Salt Inhibitor
Ammonium Salt (alkylpolyether	

Batch Searching for Data for Thousands of Chemicals

United States Environmental Protection Agency

Select Input Type(s)

- [x] Chemical Name
- [ ] CAS-RN
- [ ] InChIKey
- [ ] DSSTox Substance ID
- [ ] Exact Molecular Formula

Enter Identifiers to Search

Sodium l-glutamate
4-Hydroxy-3-nitrophenylarsonic acid
4-Nitro-1,2-phenylenediamine
Methoxypromazine
1-Phenyl-3-methyl-5-pyrazolone
1-Phenyl-2-thiourea
Phenylbutazone
1,4-Benzenediamine
Prednisolone
Probenecid

Display All Chemicals | Download Chemical Data

Select Output Format

Excel

Customize Results

- [ ] Select All

Chemical Identifiers

- [x] Chemical Name
- [x] DTXSID
- [ ] CAS-RN
- [ ] InChIKey
- [ ] IUPAC Name

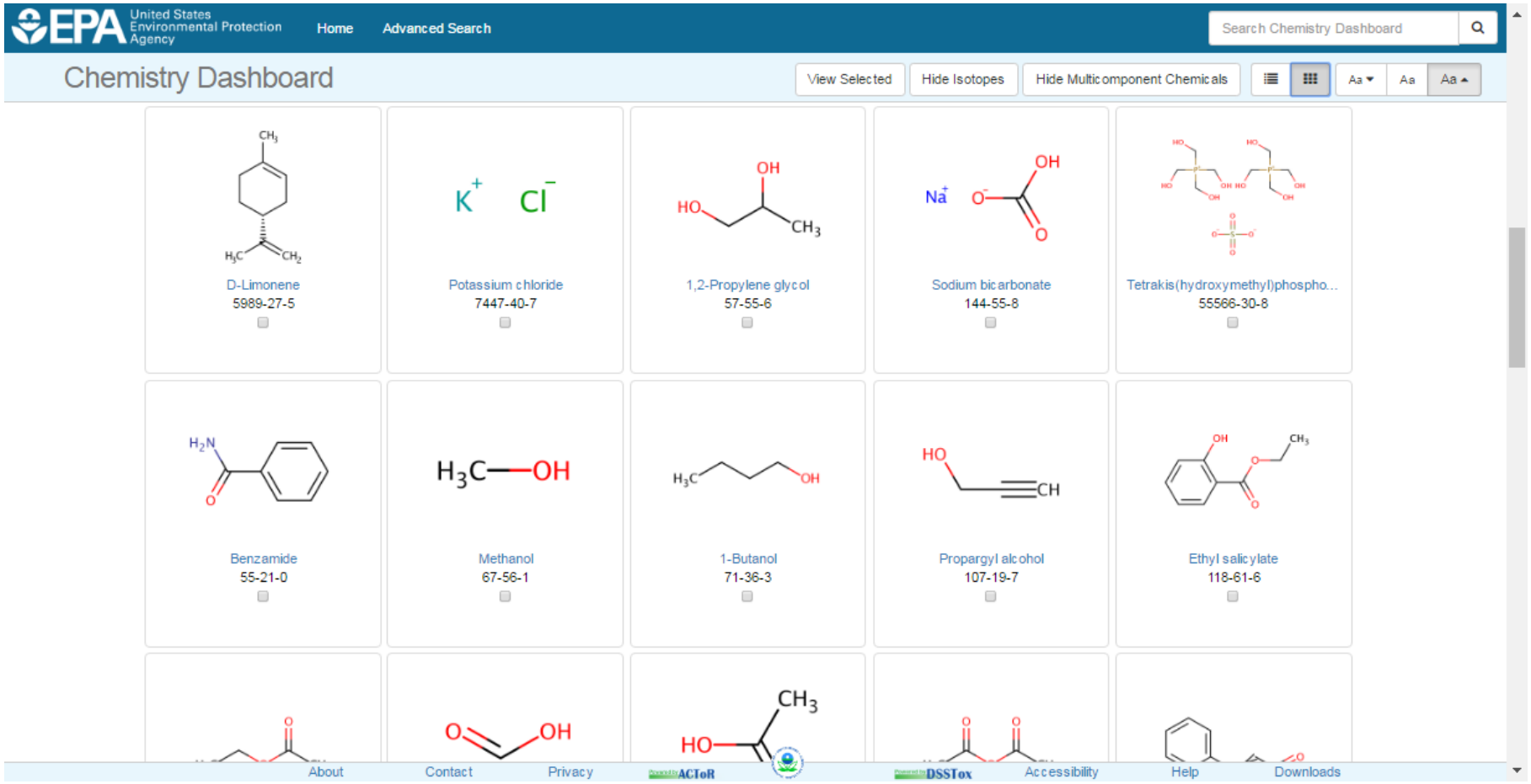
Structures

- [ ] Mol File
- [ ] SMILES
- [ ] InChI String

Intrinsic Properties

- [ ] Molecular Formula
- [ ] Average Mass
- [ ] Monoisotopic Mass
- [ ] OPERA and TEST Model Predictions

Access to associated data for review, modeling & download



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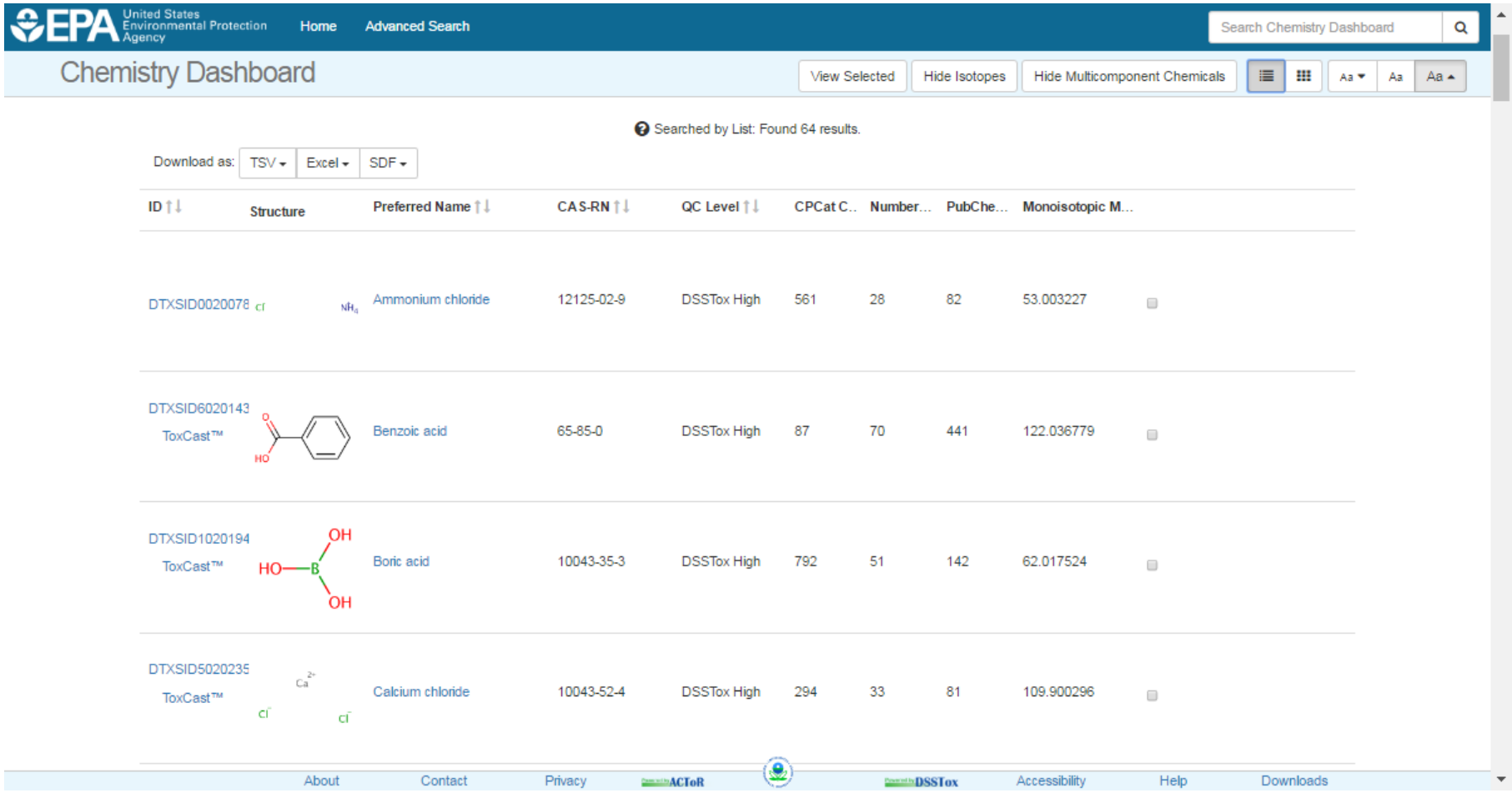
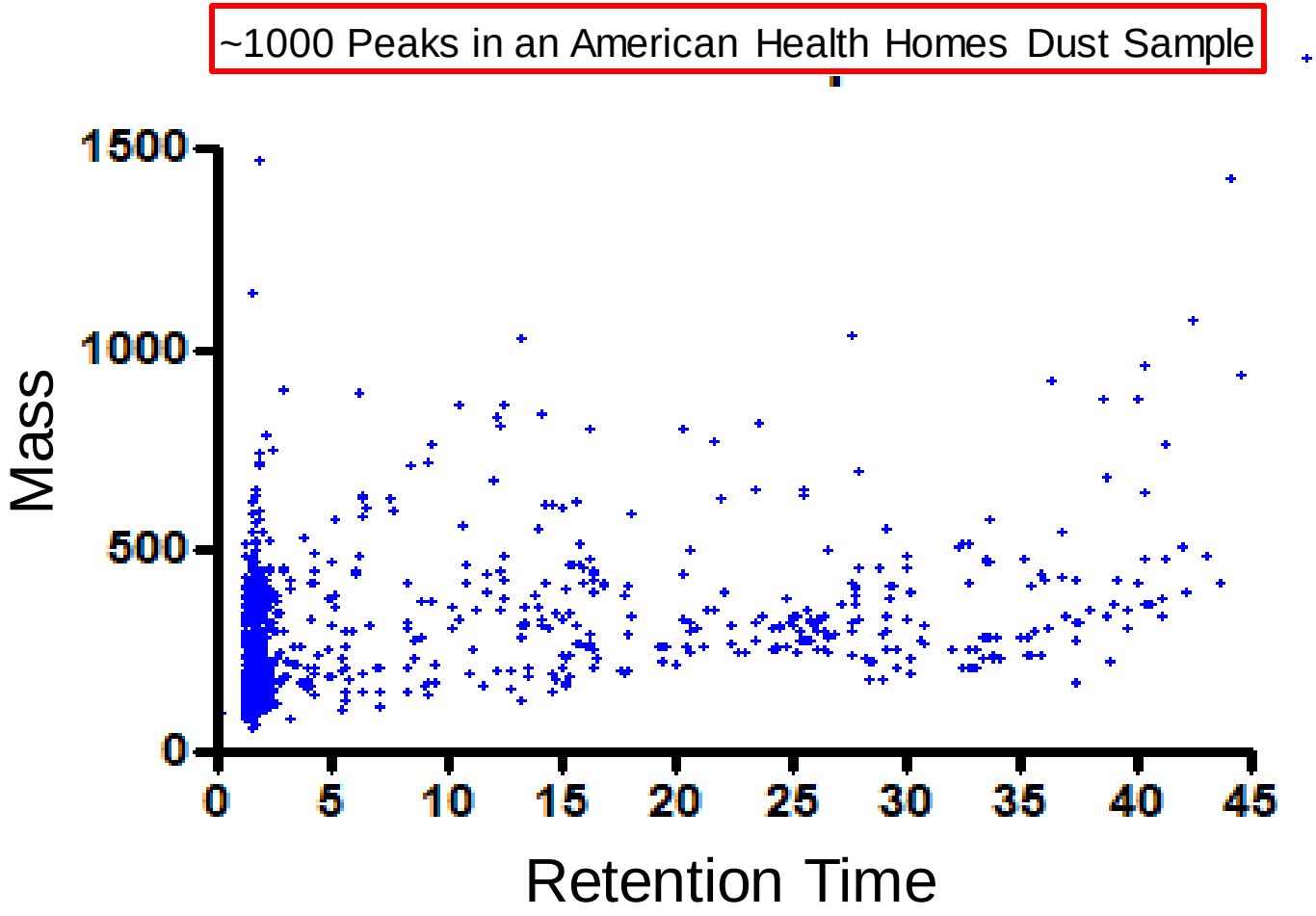


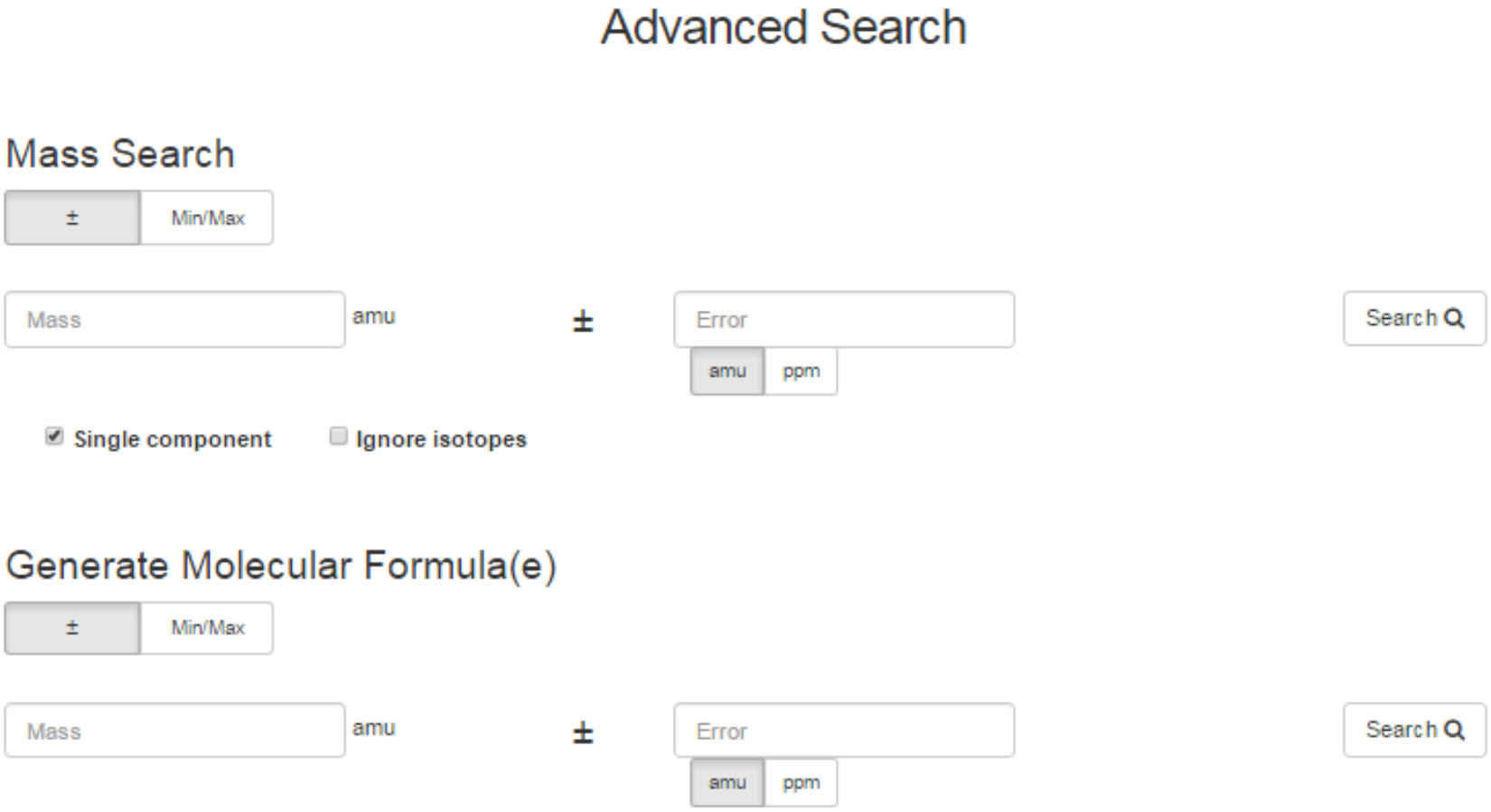
Summary Spreadsheet with Deep Links

	A	B	C	D	E	F	G	H	I	J	K	L
1	INPUT	DTXSID	PREFERRE	CASRN	DATA SOURCES	PERCENT ACTIVE CALLS	BER ACTIVE ASSAYS VS T	ACTOR REPORT	EXPOCAST I	EXPOSURE PREDICTI	NHANES	TOXVAL DATA
2	1318-09-8	DTXSID708	Libby Amph	1318-09-8	4	-	-	-	-	-	-	-
3	65195-55-3	DTXSID905	Abamectin	65195-55-3	24	-	-	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=65195-55-3	-	-	-	Y
4	526-73-8	DTXSID804	1,2,3-Trimet	526-73-8	56	0.0	0/183	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=526-73-8	-	-	-	-
5	1306-38-3	DTXSID404	Ceric oxide	1306-38-3	30	-	-	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=1306-38-3	-	-	-	Y
6	71-43-2	DTXSID303	Benzene	71-43-2	91	0.0	0/113	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=71-43-2	Y	9.13e-06	-	Y
7	100-52-7	DTXSID803	Benzaldehy	100-52-7	73	0.0	0/113	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=100-52-7	Y	3.64e-05	-	Y
8	107-05-1	DTXSID403	Allyl chlorid	107-05-1	65	1.81	5/276	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=107-05-1	Y	7.43e-08	-	Y
9	79-10-7	DTXSID003	Acrylic acid	79-10-7	64	0.0	0/64	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=79-10-7	Y	4.35e-08	-	Y
10	75-07-0	DTXSID503	Acetaldehy	75-07-0	72	22.1	61/276	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=75-07-0	Y	2.57e-06	-	-
11	116-06-3	DTXSID003	Aldicarb	116-06-3	69	4.61	31/673	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=116-06-3	Y	1.25e-08	-	-
12	68359-37-5	DTXSID503	Cyfluthrin	68359-37-5	57	6.95	49/705	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=68359-37-5	Y	1.9e-06	Y	-
13	7440-66-6	DTXSID703	Zinc	7440-66-6	44	-	-	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=7440-66-6	-	-	-	Y
14	4685-14-7	DTXSID303	Paraquat	4685-14-7	42	-	-	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=4685-14-7	-	-	-	-
15	2764-72-9	DTXSID603	Diquat	2764-72-9	31	-	-	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=2764-72-9	-	-	-	Y
16	5436-43-1	DTXSID303	2,2'4,4'-Tetr	5436-43-1	43	7.08	8/113	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=5436-43-1	Y	3.36e-07	-	-
17	60348-60-9	DTXSID903	2,2',4,4',5-P	60348-60-9	43	2.65	3/113	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=60348-60-9	Y	3.49e-07	-	-
18	68631-49-2	DTXSID403	2,2',4,4',5,5	68631-49-2	35	1.77	2/113	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=68631-49-2	Y	5.08e-07	-	-
19	108-67-8	DTXSID602	1,3,5-Trimet	108-67-8	72	0.37	2/536	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=108-67-8	Y	3.22e-06	-	-
20	12035-72-2	DTXSID202	Nickel subs	12035-72-2	30	-	-	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=12035-72-2	-	-	-	-
21	101-68-8	DTXSID702	4,4'-Diphen	101-68-8	55	2.65	3/113	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=101-68-8	Y	1.62e-05	-	Y
22	108-86-1	DTXSID502	Bromobenz	108-86-1	60	0.88	1/113	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=108-86-1	Y	2e-08	-	-
23	7790-98-9	DTXSID402	Ammonium	7790-98-9	37	0.88	1/113	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=7790-98-9	Y	6.55e-08	-	Y
24	1314-84-7	DTXSID102	Zinc phosph	1314-84-7	32	-	-	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=1314-84-7	-	-	-	-
25	557-21-1	DTXSID602	Zinc cyanid	557-21-1	18	-	-	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=557-21-1	-	-	-	Y
26	7723-14-0	DTXSID102	Phosphorus	7723-14-0	32	-	-	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=7723-14-0	-	-	-	Y
27	1929-77-7	DTXSID702	Vernolate	1929-77-7	49	1.29	7/544	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=1929-77-7	Y	6.42e-08	-	-
28	118-96-7	DTXSID702	2,4,6-Trinitr	118-96-7	48	-	-	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=118-96-7	-	-	-	-
29	540-84-1	DTXSID702	2,2,4-Trimet	540-84-1	48	0.88	1/113	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=540-84-1	Y	7.1e-06	-	-
30	112-50-5	DTXSID302	2-[2-(2-Etho	112-50-5	50	0.19	1/537	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=112-50-5	Y	4.19e-07	-	-
31	121-44-8	DTXSID302	Triethylamir	121-44-8	65	2.54	7/276	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=121-44-8	Y	2.98e-05	-	Y
32	58138-08-2	DTXSID802	Tridiphane	58138-08-2	28	-	-	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=58138-08-2	-	-	-	-
33	1319-77-3	DTXSID302	Cresol	1319-77-3	37	1.21	3/247	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=1319-77-3	Y	3.3e-05	-	Y
34	598-77-6	DTXSID302	1,1,2-Trichl	598-77-6	36	0.0	0/113	https://actorws.epa.gov/actorws/actor/2015q3/chemicalPdfExport.pdf?casrn=598-77-6	Y	9.68e-08	-	Y

Non-targeted Analysis

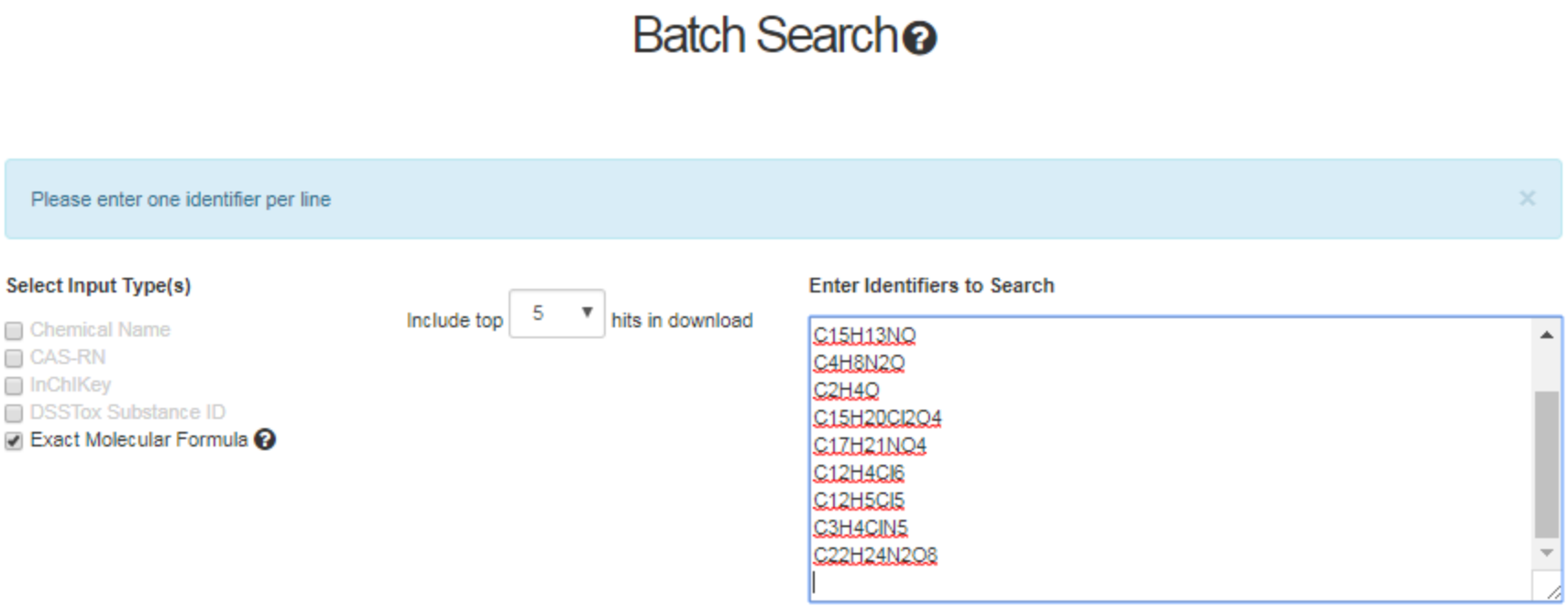


Searches for Specific Purposes



Batch Searching Formulae

United States Environmental Protection Agency



Data Available for Download

https://comptox.epa.gov/dashboard/downloads

United States Environmental Protection Agency

Downloads

DSSTox Identifier to PubChem Identifier Mapping File — Posted: 11/14/2016

The DSSTox to PubChem Identifiers mapping file is in TXT format and includes the PubChem SID, PubChem CID and DSSTox substance identifier (DTXSID).

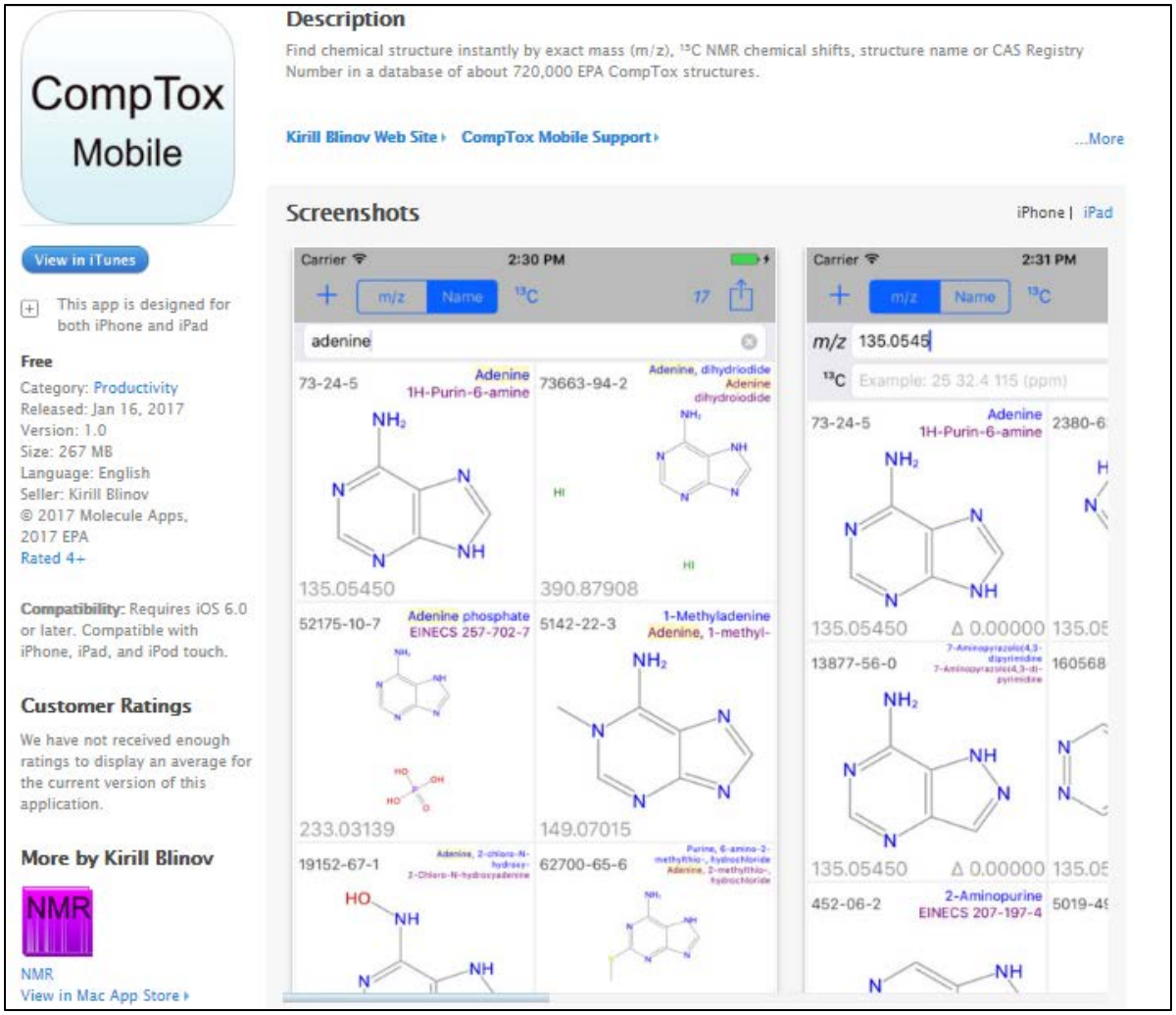
SID	CID	DTXSID
316388891	20404	DTXSID30873143
316388890	10142816	DTXSID70873142
316388889	50742127	DTXSID40873139
316388888	19073841	DTXSID20873137
316388887	11505215	DTXSID00873135
316388886	25021861	DTXSID80873133
316388885	2784427	DTXSID60873131
316388884	6731	DTXSID00873130

DSSTox identifiers mapped to CAS Numbers and Names File — Posted: 11/14/2016

The DSSTox Identifiers file is in Excel format and includes the CAS Number, DSSTox substance identifier (DTXSID) and the Preferred Name.

	A	B	
1	casrn	dsstox_substance_id	preferred_name
2	26148-68-5	DTXSID7020001	A-alpha-C
3	107-29-9	DTXSID2020004	Acetaldehyde oxime
4	60-35-5	DTXSID7020005	Acetamide
5	103-90-2	DTXSID2020006	Acetaminophen
6	968-81-0	DTXSID7020007	Acetohexamide

ca. 720,000 structures on an iPhone or iPad



Present Activities

- Update to release by end of August 2017
  - New chemical substances and structures (+11,000 chemicals)
  - Hundreds of thousands of names and predicted PhysChem Properties
  - NEW LISTS COMING SOON
    - CalEPA Office of Environmental Health Hazard Assessment
    - Agency for Toxic Substances and Disease Registry
    - Drinking Water Suspects, KWR Water, Netherlands
    - EU Cosmetic Ingredients Inventory
    - Swedish Chemicals Agency List of Substances on the Market
    - Integration to MassBank and mzCloud MS databases
    - National Environmental Methods Index
    - NIOSH Chemical Safety Cards, Skin Notation Profiles and Pocket Guide to Chemical Hazards

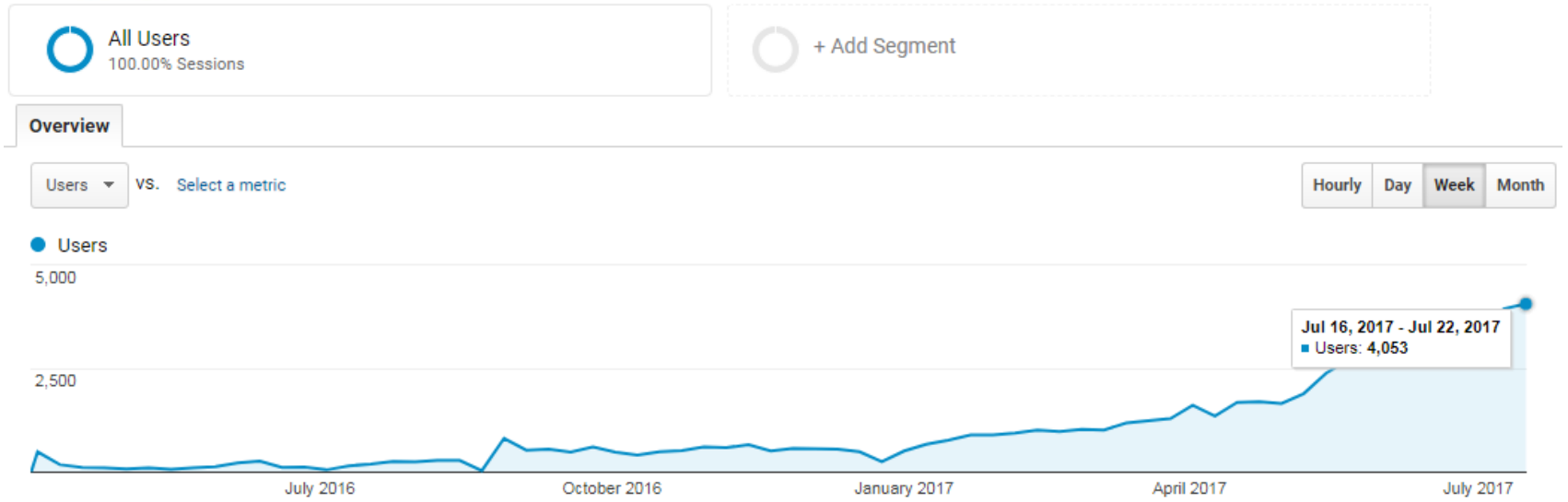
Future Work

- Continue expansion and curation of data.
- Provide “programmatic access” to all data – connect to other Agency resources and allow other scientists to integrate their scientific applications.
- Integrate algorithms that allow for real-time predictions. T.E.S.T and OPERA predictions
- Continue to assemble and enhance chemical lists and data for specific projects.

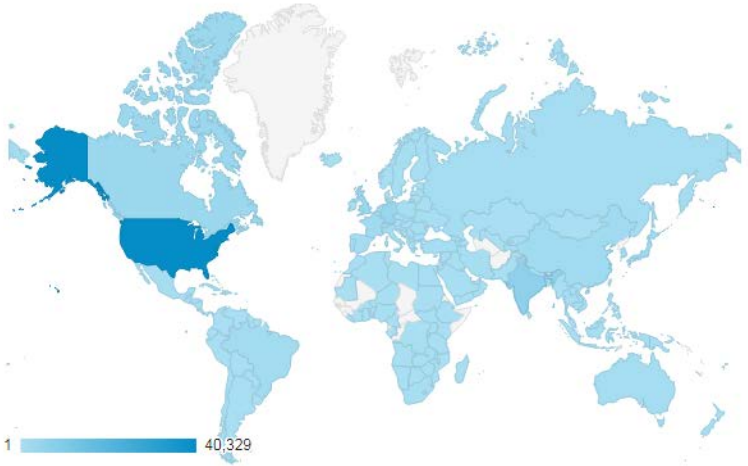
Conclusion

- The Dashboard provides access to data for ~760,000 chemicals (soon)
- An **Integration Hub** integrating multiple data sources: experimental and predicted property data, bioassay data, links to public and agency resources
- Data downloads allows for reuse in other systems and integration of resources to support research
- 1 year since initial release (on April 2016) but already an important resource we believe…

Usage Growth Statistics



Approaching 5000 unique users per week and worldwide usage



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EPA-RTP

An enormous team of contributors from NCCT

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NHERL
NRMRL

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National Center for Computational Toxicology (NCCT)

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Williams.Antony@epa.gov